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 pristine. 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

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PLENARY LECTURES

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

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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 reversibly, 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, etc.) 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
Tobin Jay Marks

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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 charge transport by specific atomistic/microstructural organization within photoactive layers and on electrodes, 3. 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.
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$_2$-$\delta$) 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$_{6-\delta}$ 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

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
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. Stojanovic, Anne M. Andrews
Email: AAndrews@mednet.ucla.edu

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 micropores 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

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Both the healing of diabetic wounds and osteoedegenerative 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 drug-resistant virus strains. In this talk, I will present ongoing work to develop a membrane-active peptide that exhibits broad-spectrum 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 combating 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 fallbacks 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 millimetre-size 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
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

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
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 », even 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 describing 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

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**HK 08**

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

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EK 01
Crystalline and Vitreous Metal Phosphates Synthesis, Structural Characterizations and Properties
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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 least, 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 $[PO_4]$ 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 $[PO_4]$ 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
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Presently used commercial lithium ion batteries (LIBs) consist of layer-type lithium cobalt oxide, spinel LiMn$_2$O$_4$ or LiFePO$_4$ as the cathode, graphite as the anode, and a non-aqueous Li - ion conducting solution or immobilized gel-polymer as an electrolyte. 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 SnO$_2$ and ternary oxides Nano-MCo$_2$O$_4$ (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.

**EK 04**

*Surface Organometallic Chemistry on MOFs and inorganic oxides for CO$_2$ and N$_2$ 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](image1.png)

**Figure 1.** MOF-based catalytic system containing Cp*Rh@UiO-67 (MOF structure UiO-67 shown in green) for the photocatalytic-reduction of CO$_2$ to formate

![Figure 2](image2.png)

**Figure 2.** a) Schematic representation of cathodic compartment for CO$_2$ 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 CO$_2$ and N$_2$, 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 H\textsubscript{2} 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

Microwave and Fluorination Treatments for Enhanced Electrochemistry of P2-type Na_{0.67}[Mg_{0.28}Mn_{0.72}]O_2 Cathode Material for Sodium-ion Batteries

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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 (MnO\textsubscript{2})-based materials. Mn is naturally abundant, and P2-type MnO\textsubscript{2}-based materials provide large tunnels for sodiation and de-sodiation processes. Sodium magnesium manganese oxide, Na_{0.67}Mg_{0.28}Mn_{0.72}O_2, 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 Mn\textsuperscript{3+}-induced Jahn-Teller distortion effect.
EK 07
1D, 2D, and 3D Electro-fabrication of Nanofiber-based Devices for Flexible Energy Storage Applications
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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.
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.

**Keywords**: transition metal oxides, layered oxides, energy storage, electrochemistry
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 intensified-charge-coupled-device (ICCD) photography imaging and Langmuir probe studies of the plasma generated by the KrF excimer laser ablation of $\text{Sm}_{1-x}\text{Nd}_x\text{NiO}_3$ 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 $2 \times 10^{-2}$ 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 $2 \times 10^{-2}$ 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 $\text{Sm}_{0.55}\text{Nd}_{0.45}\text{NiO}_3$ in the typical range used for Pulsed Laser Deposition (PLD) of complex oxides.
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

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**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.

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**NK 05**

**Green bio-synthesis of multifunctional nanoscaled oxides using natural extracts as effective bio-chelating agents**

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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 harsh 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 highly crystalline oxides and their physical properties using natural extracts as effective chelating agents. This includes TCOs, rare earth and PGMs family based oxides.

**NK 06**

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

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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.

**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, i.e., 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.

**NK 08**

*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 Co$_3$O$_4$ 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

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**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 chemo-resistive sensors.

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

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**NK 10**

**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.
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

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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

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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/diameters/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 TiO$_2$ ENMs.

The studies revealed that, the 1D nanotubular TiO$_2$, being the smallest individual ENMs possessed the highest toxicity towards *E. Coli*; further studies showed that 3D dendritic nanostructure incorporated with 1D ultrathin TiO$_2$ nanorods had the highest antibacterial efficiency. Comparative studies have suggested that, the well-engineered 3D TiO$_2$ nanomaterials (micropheres) 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), Al, 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 TiO$_2$ 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
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 continuous-flow 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+, and 1,10-phenanthroline. 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

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 fluoride-spiked water samples at fluoride concentration of 5.02mg/L and 6.4mg/L. SEM micrographs of physically coated laterite-alumina 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
WK 09
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

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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 cost 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\%.

\textbf{Keywords}: zeolite, natural, water, purification, heavy metal
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 nutrient 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 of added carbon and nutrients and impacts on soil organisms should be considered.

Keywords: biofertilizers, biowaste, biomass
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 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
Translating Africa’s comparative advantages in minerals into competitive advantages in materials
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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

Mining contribution to the Botswana economy through local content
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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. Substitution 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
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.
CK 01

Application of Molecular Structure Methods to Materials Problems

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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.

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

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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 self-assemble 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 interfacial free energy 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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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 MnO\(_2\), TiO\(_2\). 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

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**CK 05**

**Dusk of Moore’s Law: opportunities for HPC and materials science?**

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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 diverse 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 deficienc, 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
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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

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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

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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 web-seminar is arranged involving a U.S. researcher (live online), the students and their lecturer. Activity photos are taken and posted on the project websites: www.scibridge.org; www.facebook.com/scibridge; 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
My basic thesis is that we need to train globally-competitive and locally-relevant engineers in the 21st Century. In the talk, I would define some of the salient issues confronting Engineering Education in most SSA countries. I will then discuss potential resolution strategies. In doing so, I will go beyond the usual complaint of lack of funding. And yes, funding is needed, but we need much more valuable commodity – innovative ideas and approaches to engineering education. In order to adequately completely the problem, we must discuss the environment, just like in In Thermodynamics, you can only define the system as a subset of the environment. The environment influences the behavior of the system. So, the first thing that we must do is to look at the global imperatives for engineering education in the 21st C. I will then explore today’s global landscape and will discuss some of the imperatives for engineering education and the need to think globally and to be globally engaged in the 21st Century – the so-called global century. I will then address those imperatives within the African context.

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

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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 electrochemical 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 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 $1.9 \times 10^{-7}$ M and $3.1 \times 10^{-8}$ 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)

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 G0/G1 block. However, in combination with proton radiation, a G2/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
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 reticu-la-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.

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 CuInS₂/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)

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**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 10⁸). 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.

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**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 (H₂O₂) 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

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**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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Graphene oxide (GO) is a two-dimensional (2D) materials with fascinating properties such as large surface-to-volume 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), micro-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-diffusion 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. Three-dimensional 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 ±12 µm. 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 fibre-gelatin 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
**HO 12**

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

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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 micro-porous 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 are 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
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.

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 bi-functionalized 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).

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**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

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**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-carbonaceous 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)

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**HO 21**

**Extraction and Characterization of Chitosan from Black Soldier fly (Hermetia 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*<sub>max</sub>) 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<sub>max</sub> 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

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**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 $5.98 \times 10^{-3} \mu M$ to $62.8 \mu M$ with detection limits 118, 129 and 166 nM for GCE/MWCNT-NiO, GCE/MWCNT-ZnO and GCE/MWCNT-Fe$_3$O$_4$ 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 (αVβ3, αVβ6, αVβ8) 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
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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
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 Phyto-formulations 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 Nano-optimised 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

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

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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. It 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, high-resolution 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 pdI of 0.598 and zeta potential of -7.87±4.35mV. At pH 2, the nanoemulsion released 76 ± 2 % of nevirapine within 2 h, while at pH 6.4 value representing the small intestine, amount of nevirapine released was 41.6±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.
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. Macrosmoothness was 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 multi-component 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

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**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 \(\text{SO}_x\) and \(\text{NO}_x\) 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.
EO 03

Hydrogenation of Ti-based Quasicrystalline Powders Produced by Mechanical Alloying

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Icosahedral (i) quasicrystals, which have a new type of translational long-range order and display non-crystallographic 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 rapid-quenching 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 i-phase 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
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 so-called 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 core-shell 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.

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**EO 05**

**Elastic Properties of Strontium difluoride single crystal by means of Brillouin Scattering**

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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 (ΩA) scattering (RIΩA) technique is introduced. In this geometry, we can simultaneously obtain RIΩA 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

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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.
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.

Design of Materials for Advanced energy storage
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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 binder-free 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
EO 10
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 to 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⁻¹ upon 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
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 ruthenium-based 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

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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.
**EO 14**

**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 Al and Cu doped ZnO (AZO and CZO) thin film electrodes. The concentration of Al 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.% Al 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 Al 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**

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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 graphene 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
EO 16

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) tri-metallic 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 tri-metallic 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

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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
**EO 18**

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  

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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, SnO$_2$ and Fe$_2$O$_3$), 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
**EO 20**

**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 Ab-into 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 ultimately battery performance. 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**

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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 sun’s 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
EO 22

Novel photocatalytic materials for hydrogen production

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TiO₂ 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 end uses. 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 (Thermo-gravimetric 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, Thermo-gravimetric Analyser, Ansys software

Zinc Oxide nanorod structures grown by chemical bath deposition on a seed layer prepared by a successive ionic layer adsorption and reaction (SILAR) method
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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 underlaying 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 A/g (1.7 mA/cm²).

Exploring the YₓBi₂₋ₓO₅ 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. SOFCs are, however, marred by a variety of limitations 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 (Fm₃m) to lower temperatures by means of yttria doping. These attempts have been successful; various YₓBi₂₋ₓO₅ members have been found to display the Fm₃m structure at room temperature.

Keywords: SOFC, PXRD, electrolyte
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 micrometer-period, 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

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**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. A good cathode material should include thermal and chemical stability, high capacity, affordability and low toxicity. 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 borophosphates 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

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**EO 30**

**Sulfur cathode materials for lithium–sulfur batteries**

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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

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**EO 31**

**Catching the sun at low cost**

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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
 EO 32

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-known 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

Ab-initio simulations of photocatalysts for hydrogen production
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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
**EO 36**

**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 market because of its large-scale energy storage potential applications. Moreover, Zn has various outstanding properties such as reasonable redox potential, high safety, low cost, most abundant and 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-MnO₂:nanorods 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 more so 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
EO 38

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-Fullerene (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 UV-stability 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 CuAlS2 thin films deposited by chemical-bath deposition.

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CuAlS2 has recently gained interest as an alternative earth-abundant absorber material for thin film solar cells. CuAlS2 belongs to Group I (ternary chalcopyrites) of ternary ABX2 semiconductors, which consists of the ABrX2VI compounds where A=Cu, Ag; B=Al, Ga, In; and X=S, Se, Te. CuAlS2 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 CuAlS2 are earth abundant, inexpensive and environmentally benign. Several methods have been utilized for preparing ternary chalcopyrite CuAlS2 such as chemical spray pyrolysis, chemical bath deposition, spark plasma scattering, metal decomposition, iodine transport, single source thermal evaporation deposition. This work reports CuAlS2 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 50°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$_2$Al$_2$S$_4$ 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 (Q-PPO/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 ($^1$H 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
EO 42

Comparative performance of non-conventional Ga\textsubscript{1-x} In\textsubscript{x}NyAs\textsubscript{1-x} sub-junction for tandem solar cells

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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 Ga\textsubscript{1-x} In\textsubscript{x}NyAs\textsubscript{1-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 \cite{1}. The minority carrier lifetimes observed in Ga\textsubscript{1-x} In\textsubscript{x}NyAs\textsubscript{1-x} are often less than 1 ns \cite{2}, which is 500 times less than typical GaAs minority carrier lifetime \cite{4}. The short minority carrier lifetimes result in very short diffusion lengths that make it a challenge to design the Ga\textsubscript{1-x} In\textsubscript{x}NyAs\textsubscript{1-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 Ga\textsubscript{1-x} In\textsubscript{x}NyAs\textsubscript{1-x} solar cells. In this letter the relative performance of Ga\textsubscript{1-x} In\textsubscript{x}NyAs\textsubscript{1-x} /GaAs junctions’ solar cells of different designs is studied. Performance parameters reported are: temperature coefficients of efficiency and dark current.

Keywords: Ga\textsubscript{1-x} In\textsubscript{x}NyAs\textsubscript{1-x}, dark current, solar cell, efficiency

EO 43

Improving the Photooxidative Stability of Organic Photovoltaic Technologies

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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.\cite{1} Here we present a detailed study of the photooxidative degradation of organic photovoltaics based on two widely used benzodithiophene-co-thieno[3,4-b]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.\cite{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)MnO$_3$, a canonical solid oxide fuel-cell (SOFC) cathode material, and for (La,Sr)(Co,Fe)O$_3$, 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 Electro catalysts 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 TiO$_2$. Using this method, we are able to improve the overpotential of an IrO$_2$ 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 RuO$_2$ catalysts were improved by 300 mV for OER with deposition of thin layers of TiO$_2$. 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

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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 – 139.3 eV 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\(_{1-z}\)S\(_z\) 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 TiO\(_2\)/In(OH)\(_x\)/PbSO/PEDOT:PSS/Au has been fabricated and has shown the following parameters: \(V_{oc} = 0.28\) V, \(I_{sc} = 7.4\) mA/cm\(^2\), \(FF = 0.4\) 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.

Nanomechanical and Morphological Characterization of solution-processed MoO\(_3\) 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 (sMoO\(_3\)) and poly [2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene]) (MEH-PPV) thin films and their interface for OLED applications. The sMoO\(_3\) 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 sMoO\(_3\) and MEH-PPV films. Nanoindentation of the sMoO\(_3\)/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: sMoO\(_3\), Nanoindentation, Morphology, OLED.
NO 01

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 loxes. 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 future recording media. The systems under study are nanoparticles of Fe2O3, MnFe2O4, MnCr2O4, Cr2O3, Fe3O4, CoCr2O4, other core-shells and their alloys. The work seeks 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 control 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

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**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
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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 employed as tools to characterize the isotopic nickel thin films Fabry-Perot resonator. Polarized 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 be 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

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

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**NO 07**

The effect of N-configurations on the detection of dopamine at N-doped graphene-modified 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 dopamine (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 N-configurations. 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 µM, 2 – 150 µM, and 4 – 40 µM, with the estimation of the detection limits (S/N = 3) determined to be 0.131 µM, 0.153 µM, and 0.645 µM at the NGr-2/ITO, and NGr-10/ITO and NGr-20/ITO electrodes, respectively. Thus, the NGr-2/ITO electrode exhibited 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. Additionally, the enhanced heterogeneous electron transfer rate constant at the NGr-2/ITO electrode (k = 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.

**Scheme 1:** 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 La$_2$O$_3$-CuO-Co$_3$O$_4$ 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 Co$_3$O$_4$ are p-type narrow band gap semiconductors whereas La$_2$O$_3$ 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-Co$_3$O$_4$-La$_2$O$_3$ ternary mixed oxide nanostructures with different La$_2$O$_3$ 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 Co$_3$O$_4$ and hexagonal La$_2$O$_3$ crystallographic phases. These phases were confirmed through XRD and Raman studies. Increasing the La$_2$O$_3$ content beyond 10 % resulted to reduced intensities of the CuO and Co$_3$O$_4$ 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 La$_2$O$_3$ additive.

Keywords: nanostructures, La$_2$O$_3$-CuO-Co$_3$O$_4$, mixed oxide, hydrothermal, gas sensing

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. 4×10-16 m$^{-2}$. 

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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 µm 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

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

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Nanotechnology has proved to be an important field of modern study looking at design, synthesis, and manipulation of particle structures ranging from approximately 1-100 nm. Silver has long been used as antimicrobial substance in various applications without posing threats to human health or the environment. The reduction in the size of the bulk silver to nano scale has brought with it several novel properties that could prove very useful to modern day society. Research was carried out to show at which particular concentration and at what proportion the nano silver was needed as an additive to create an effective product that is also cost effective. The method used to synthesise the nano silver was reduction by a suitable agent. The product was characterized using Fourier Transform Infrared Spectroscopy (FTIR) for chemical composition, ultraviolet-visible spectroscopy(UV-VS) for size range, the antimicrobial test was an inhibition zone test using a suitable agar and bacterial strain. The results showed that the product was effective at concentration of 0.0015mol/dm3 as evident by the effective zone of inhibition. This research seeks to take advantage of the novel properties of nano silver, the antibacterial nature of nano silver to be precise and making use of this property to create a highly functional antibacterial paint for use in high microbial risk areas such as hospitals and areas like food processing industries in an effort to lower the contamination of things handled in these areas and remove the walls as a source of bacterial contamination.
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.

NO 13
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
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The increasing global thrust towards sustainability has led to the use of natural fibres or recycled fibres (obtained from various forms of waste paper) as reinforcements for the production of cement-based composites. This has led to a new approach for the industrial design of products and processes along with the implementation of sustainable manufacturing strategies to "optimize the total recycle of waste materials". Developing countries such as Nigeria possess abundant but underutilized biomaterial resources which can be harnessed for the production of sustainable building materials. This paper presents the production and characterization of fibre cement composites using recycled fibres obtained from waste newspaper and carton boxes. A slurry-dewatering process (a crude reproduction in small scale of the Hatschek Process) was used to produce fibre-reinforced cement pads with 10% by mass fraction of fibres. The composites were characterized based on physical, microstructural and mechanical (flexural strength) properties. Apparent Void Volume (AVV), Bulk Density (BD), and Water Absorption (WA) of the composites were obtained and characterized in accordance with ASTM C1185. The microstructural analysis of the Scanning Electron Microscope (SEM) images revealed a more homogenous distribution of fibres in the composites reinforced with waste newspaper fibres compared to carbon box fibres. A 3-point bending configuration was used to determine the Modulus of Rupture (MOR) for each composite. The average MOR for the saturated newspaper fibre reinforced-composites obtained was 5.80 MPa at 14 days which satisfied the minimum saturated MOR requirement (5.50 MPa) for non-asbestos fibre cement roofing products as specified in ASTM C1225-04. On the other hand, the average values for the carton box fibre reinforced composite was slightly lower (4.58 MPa). However, both composites met the ASTM C1186-02 minimum requirement of 4.00 MPa for Grade 1 fibre cement sheets. The result of this study demonstrates the potential of the use of recycled natural fibres for the production of mechanically robust and sustainable non-load/low load bearing building elements.

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-of-concept-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 high-temperature 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 ALD-grown MoS₂ samples) and the proposed surface coordination chemistry mechanism at hand.
We report on simple method for the formation of transition conducting metal oxides (TCMOs) like pure SnO$_2$, ZnO nanoparticles, and a SnO$_2$/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 wurzite 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 (0 0 2) 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 O$_2$ 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 O$_2$ 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 SnO$_2$/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, SnO$_2$, ZnO, XRD, HRTEM, Field Emission, Sensors
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

Catalytic soot oxidation using ceria and copper nanocomposites
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Nanosized CeO₂-CuO (CeCu, 2:1) and CeO₂-CoO (CeCo, 2:1) were synthesized by co-precipitation from nitrate precursors using 25% ammonia solution (NH₄OH) as the precipitating agent. The catalysts were calcined in air at 800°C for 4h to evaluate the thermal stability. Powder x-ray diffraction (XRD) and Dynamic Light Scattering (DLS) techniques were used for catalyst characterization. A Thermo gravimetric/Differential Thermal Analyzer (TG/DTA) was used to determine the catalytic efficiency and soot oxidation activity. Ce-composite nanoparticles heightens the redox properties of the catalyst relative to undoped ceria. The Ce-composite samples exhibited excellent soot catalytic combustion performance by decreasing activation energy of soot oxidation.

Key words: soot oxidation, catalytic combustion, CeO₂-CuO, CeO₂-CoO, co-precipitation
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.

NO 20
Radionuclide liquid wastes treatment of $^{68}$Ge 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 $^{68}$Ge 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 coeffient (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, $^{68}$Ge radionuclide, Graphene, Graphene oxide, Sorption
**NO 21**

Surfactant-free, aqueous dispersions of carbon nanomaterials

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Keywords: Graphene, SWNTs, KCs, Reductive dissolution, hydrophobicGraphite intercalation compounds can be readily exfoliated down to single layers in aprotic solvents due to the favorable entropic contribution of dissociating counterions, yielding graphenide solutions. The resulting graphenide solutions are prone to re-aggregation after oxidation and must be handled in a dry, oxygen-free environment. In this contribution we show that homogeneous air-stable dispersions of single layer graphene in water with no surfactant added can be obtained by mixing air-exposed graphenide solutions in tetrahydrofuran (THF) with previously degassed water and evaporating the organic solvent. \textit{In situ} Raman spectroscopy of this single layer graphene in water show bands at 1343, 1586, 1620 and 2681 cm\(^{-1}\) corresponding to the D, G, D’ and 2D bands of graphene respectively. The 2D band at 2681 cm\(^{-1}\) is well fitted with a sharp lorentzian line (∼28 cm\(^{-1}\)) which is a hallmark of single layer graphene. Coatings on glass substrates from these graphene dispersions have conductivities of up to 30 kS/m. Recent results on surfactant-free and stable single walled carbon nanotubes (SWNTs) dispersions in water and their application as transparent electrodes in transparent and flexible supercapacitors and organic solar cells will be presented.

**NO 22**

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 E\(_{2g}(h)\) 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 its 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 Infra-red Spectroscopy (FTIR), Photoluminescence spectroscopy (PL), and photocatalysis were carried out.

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

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 fluxes, 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 was also presented in this research work. In-addition, the stability of wurtzite structure under ions 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.
Vanadium dioxide (VO$_2$) 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 VO$_2$ based SRD decreases the request of spacecraft power budget. As an active SRD, an ideal VO$_2$ 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 VO$_2$ 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 VO$_2$ 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 VO$_2$ 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 VO$_2$ 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 VO$_2$ metallic phase. From the XPS measurements of V2p and O1s core level spectra, an oxidation of vanadium from V$^{4+}$ towards V$^{5+}$ 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 neutron-induced 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 VO$_2$ 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 VO$_2$ 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 nano-scale 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 papilionid 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

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

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Today, the innovative development in electrospinning technology enables nanofibers to be produced at industrial scale. This development translated into significant competitive, environmental and economic benefits to manufacturers in several industries. The superior properties of nanofibers such as high specific surface area, inter-connected pore structure, surface functionality and high porosity create a new value for currently used flat materials, and have been integrated into a wide range of commercial applications including various segments of air filtration, liquid filtration, wound dressing, tissue scaffolds, waterproof and breathable membranes. Elmarco’s needle–free Nanospider™ technology is well recognized by industry leaders for providing excellent web and fiber uniformity, high productivity, and ability to consistently meet key performance characteristics. Laboratory tools are designed in the way that enables complex development of nanofibrous layers made of broad range of polymeric solutions and offers variability in settings. Laboratory tools use the same stationary electrode system as found in industrial Nanospider™ Production Lines, therefore the results from experimental work are easily upscalable to the industrial high volume manufacturing. Ability of spinning a variety of polymers and wide range of substrate materials capability make Nanospider™ technology an effective tool for nanofiber material integration across numerous industrial applications.
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

Effect of Particle Size of Pozzolanic Addition on the Properties of MgO-based Cement

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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% SiO\textsubscript{2}) for early and later strength of 7 and 28 days were determined by varying the particle size of the RHA at 425 μm, 150 μm, and 106μm 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 μm 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

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**NO 30**  
**Structural and optical properties of MgXZn\textsubscript{1-X}O (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\textsubscript{X}Zn\textsubscript{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\textsubscript{X}Zn\textsubscript{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\textsubscript{X}Zn\textsubscript{1-X}O, Nanomaterials, stacking faults, alloy broadening

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**NO 31**  
**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 (Al\textsubscript{2}O\textsubscript{3}, MgO, SiO\textsubscript{2}) 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

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

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Cuprous iodide (CuI) is a p-type transparent halide semiconductor which received the earliest research interest among its family members; CuCl, CuBr, AgCl, AgBr and AgI. 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 CuI 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 CuI 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 CuI 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.

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 moiety 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 oleylamine (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

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**NO 34**

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

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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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**NO 35**

**Green Synthesis of CePO₄ Nanomaterials via Callistemon viminalis Extract**

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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

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

Nanomaterials Industrial Development Facility (NIDF): Crossing the innovation chasm

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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

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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 apart from tampering with their dimensions. This can be advantageous in cases where the nanostructures must have specific dimensions corresponding to specific energies of excitation.

Keywords: Nanostructures, electric confining potential

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 respectively. It was also observed that the particle sizes of the nanoparticles increased as the 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

Immiscible Polylactide/Poly(ɛ-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(ɛ-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
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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
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) \(\text{N-alkyl-N-ethanoldithiocarbamate}\) 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

Investigating the anionic polymerization of aldehydes, promoted by strong organic bases
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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 (Tc), significantly below room temperature; e.g. for PPA, Tc = -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 upsurges 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

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 nitrogen-doped nanotubes (NCNTs) were synthesized using a CaCO3/Co-Fe catalyst in a CVD reactor and then functionalized in aqua regia. 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 adsorption-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

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**NO 51**

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

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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.

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**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 $5 \times 10^6$ V.m$^{-1}$ and for a given disorder amount.

**NO 53**

*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 ($iHCn$), 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 $iHCn$, 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% H$_2$SO$_4$ solution at room temperature.

**Keywords**: nano-sized, high purity graphite, flotation concentrates
Synthesis and thermal conductivity enhancement of silver nanowires dispersed ethylene glycol-based 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 reductant, 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°C. Remarkably, enhancement up to 23% in thermal conductivity of AgNWs:EG nanofluid aged for 5h was found compared to EG base fluids. We observed a nonlinear relationship between thermal conductivity and volume fractions, and also the existence of a strong temperature effect on this anomalous thermal conductivity enhancement.

Keywords: Nanofluid, silver nanowires, thermal conductivity

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 in situ 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
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 Au⁰ 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

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 $^1$H, $^{13}$C and $^{15}$N 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 µM.

**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 (Eu$_2$O$_3$) 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(NO$_3$)$_3$.5H$_2$O) salts as a precursor. Eu$_2$O$_3$ 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 Eu$_2$O$_3$ 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 ($^{5}$D$_{0}$–$^{7}$F$_{3}$).

**Keywords**: Biosynthesis, *Hibiscus sabdariffa*, Eu$_2$O$_3$ nanoparticles, Rare earth oxides, Luminescence
WO 01
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 systems 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 Ileret, 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. Deflouridation 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
WO 03
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 (ΔH), entropy (ΔS) and Gibb’s free energy (ΔG) 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
WO 05
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 l/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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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 value-added 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 bio-concentrate 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)
WO 09
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 integrated 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 (Cd²⁺) from waste-water. Membranes were prepared via an interfacial polymerization (IP) using hyperbranched-polyethyleneimine (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 85.88⁰, however after HPEI grafting the contact angle decreased to 26⁰ 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, Cd²⁺ 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 Cd²⁺ 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 Cd²⁺ or metal precipitation in basic solution. Adsorption data showed that the adsorption capacity of PES/HPEI membrane for Cd²⁺ is higher than that of pristine PES.

Keywords: Cadmium, Nanofiltration, Thin film composite, Hyperbranched polyethyleneimine, Anodic Stripping Voltammetry.
Electrophoretic Deposition of TiO$_2$ 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 (TiO$_2$) 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 TiO$_2$ particles to the substrate with homogeneous film coatings, is ethanol, a TiO$_2$ 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 TiO$_2$ thin films decreases exponentially with the ultraviolet light (UV) illumination time and it is also dependent on film thickness, and sintering temperature of the TiO$_2$ thin films. Highest rate of photocatalytic activity is observed at an optimal film thickness of 95.0 ± 2.0µm sintered at 300.0 ºC. 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

Downscaling the conventional iron barrier technology to safe drinking water

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Fe$^0$ 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 Fe$^0$ filters. Metallic iron-based filters (or Fe$^0$ filters) have a great potential for decentralized safe drinking water provision. However the whole effort to estimate the long-term performance of Fe$^0$ filters should be reconsidered since the whole literature on metallic iron (Fe$^0$) for water treatment is based on the false premise that Fe$^0$ is a reducing agent. Accordingly, Fe$^0$ oxidation by water has been wrongly considered as a side reaction. This work deals with the filtration of aqueous contaminant in a Fe$^0$ 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-Sørensen 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

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 1ℓ 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

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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 time-dependent 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
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
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 photocatalytic degradation of chlorophenols in water. The synthesis was done using zinc nitrate hexahydrate (Zn(NO$_3$)$_2$. 6H$_2$O) precursor and sodium hydroxide (NaOH). Silver nitrate (AgNO$_3$) was added to ZnO and reduced with sodium hydroxyde to produce the silver nanoparticles within the ZnO structure. The silver content was varied from 1, 3 and 5 wt% for optimisation. The nanocomposites were characterised using ultraviolet - visible spectroscopy (UV-Vis), photoluminescence (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 photohocatalytic 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

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**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 pseudo-first, 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
WO 22

Bio-adsorbent from avocado peel for removal of As\(^{3+}\) and Cd\(^{2+}\) 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\(^{-5}\) \(\mu\)A while Cd(II) in 10 ppm standard solution decreased from 3x10\(^{-5}\) to 5x10\(^{-6}\) \(\mu\)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**

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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 fluoride-co-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

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
WO 27
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–hydroxyapatite 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.
WO 29

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 activated carbon are employed in the design of efficient and effective water filtration membranes capable of eliminating pathogens and viruses from water. The DE waste 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

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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
WO 31

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/2,5-diaminobenzenesulfonic 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
WO 33
Dual-Functional Ultrafiltration SiO$_2$ 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 (ClnP-PPy-Fe$_3$O$_4$) nanocomposite as a potential adsorbent for Cr(VI) and V(V) was prepared via polymerization of pyrrole monomer using FeCl$_3$ oxidant in aqueous medium in which clinoptilolite-Fe$_3$O$_4$ 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
WO 35

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 ~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

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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(III)) 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 (≥56 %) accounted for the bulk of cations removal on the BMF-0.5 composite, while adsorption on pores or within various partitions was dominant (≥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 adsorbents and increase in temperature enhanced adsorption to an extent: 298>288>308 K. The adsorption capacities of BMF-0.5 and BMF-1 for both
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

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**WO 37**

*Quaternary imidazolium-modified montmorillonite clay for disinfection of water*

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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*

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**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-trichlorophenol (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° ±1.25) compared to the pristine PES membranes (55.70° ±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

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**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 Co₃O₄. The size of the nanoparticles decreased with an increase in the amount of H₂O₂ added and the shape was found to be cubic as determined by TEM. The catalytic properties of the obtained Co₃O₄ 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

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**WO 40**

**Visible-light-induced BiVO₄ semiconductors for efficient wastewater treatment**

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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*

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**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) colorimetric 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 self-assembles in nano- to micro-meter thick membranes upon dip coating. The so formed thin films modulate mass transport (e.g. O2 and CO2 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 O2 and CO2 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 a 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
AO 03
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 in 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 thuringiensis 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

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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 clearly 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

Bio-based nanostructures for food applications

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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
AO 07

“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 μm 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

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Nowadays, packaging has become an essential technology in the treatment and commercialization of food, slowing the food spoilage while improving the safety in the food consumption. Plastic materials have become more important due to their excellent properties for this type of applications (transparency, flexibility, versatility, low cost, ease of processing, heat sealing, tunable and/or selective permeability to mass transport, etc.) and its wide variety of formulations, which allows tailor-made structures for specific applications. However, the increase in the use of plastics for packaging applications has resulted in an environmental problem, mainly due to their non-renewable origin and the extremely slow degradation rate.

Recently, due to the environmental policy being imposed worldwide, a considerable industrial interest in using renewable and biodegradable polymers as an alternative to oil-based conventional plastics has arisen. The use of biodegradable and renewable polymers would allow the treatment of the package after its use as an organic compostable residue, therefore contributing to the reduction of polymeric solid waste destined for landfill or avoid permanent pollution in case of direct release to the environment.

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Some of the most promising and common renewable polymers are "food-competitive", i.e. they are obtained from food sources (e.g. thermoplastic starch and lactic polyacid). This fact may pose a moral conflict should the use of these materials become massive and their cost decrease to the commodity range. In this sense, there is a family of renewable biopolymers whose origin comes directly from bacteria, the so-called polyhydroxyalkanoates (PHA). These materials, as being polymers derived from microorganisms, would fall out of the debate granting them a competitive advantage from the point of view of industrial social-environmental introduction [4]. However, these materials still present some limitations for their direct applicability in a massive industrial scale, particularly in the field of food packaging [5]. In this contribution, several strategies devoted to improve the industrial applicability of PHBV to the packaging sector will be explored. All the strategies have been developed from a clear technical feasibility perspective, as well as of a simple applicability in an industrial environment.

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
Small, synthetic single stranded oligonucleotides (ssDNA/ssRNA) known as aptamers are capable of binding non-covalently 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 result 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 agro-waste 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
AO 13

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
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 microparticles 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 thiourea was confirmed by the SEM-EDS analysis of the materials after Pd(II) elution. Palladium loading capacity of the functionalized silica resins were in the order S-NSN (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 workplace 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
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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 metallurgy 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 cracked surface. The findings indicate that the unstabilized ferritic stainless steel is resistant to solidification cracking compared to the stabilized steel.

Keywords: Houldcroft, ferritic stainless steel, gas tungsten arc welding, microstructure
Leveraging People, Process, and Data to Advance the Large-scale Deployment of Sustainable Structural Materials

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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 science-driven 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

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**

**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 (C₂₄H₁₂) 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 07**

**Effect of concrete quality on the sensitivity of the chloride conductivity test to salt concentration and capillary voltage**

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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

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**MO 08**

**Exploration of local Cellulosic fibers, Modification and potential use for the local Industry**

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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 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 09

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 thousands year 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 10

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 11
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 12
Addressing Africa's development challenges through use of waste materials in concrete
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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 13

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 (C24H12) 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 14
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, Energy-dispersive 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 15
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 16

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.
CO 01
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
CO 03

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
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 calculated from 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

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 carbonitrides 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
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With the recent scenario of affordable computers with large RAM and storage capabilities as well as the 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 sharpening 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 state-of-the-art 
\textit{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.

\textbf{Keywords:} DFT, VS$_2$, Batteries.

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, dithiocarbamate and dithiophosph ate) 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.

\textbf{Keywords:} pyrite, surface, water molecule, thiol collector, adsorption
CO 11

Effect of transition metals clusters on the electronic and magnetic properties of MoS$_2$

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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 MoS$_2$ 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 MoS$_2$. The calculated clustering energies shows that TM ions exhibit dispersive distribution void of cluster formation in MoS$_2$ lattice. Generally, there is a reduction in the electronic band of doped MoS$_2$ compounds with a consistent red shift in the absorption spectra. The calculated redox potentials of H$_2$O splitting lie properly astride the valence and conduction bands for Cr doped MoS$_2$, 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 NaMn$_2$O$_4$ and MgMn$_2$O$_4$ polymorphs

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Spinel lithium manganese (II) oxide (IV) (LiMn$_2$O$_4$) 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 NaMn$_2$O$_4$ and MgMn$_2$O$_4$ 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 NaMn$_2$O$_4$ and MgMn$_2$O$_4$, 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 ReSe$_2$: A theoretical investigation

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Effect of pressure on structural, electronic, mechanical, and Dynamical properties of ReSe$_2$ 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 ReSe$_2$ 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 ReSe$_2$ 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 ReSe$_2$ to large pressure the material becomes somehow more compact due to reduced inter-atomic distance hence increase in magnitude of elastic co_e_cients as well as bond strength. The Dynamical instability was investigated by computing the phonon frequency to check for imaginary modes. ReSe$_2$ is dynamically stable below 40 GPa. The band gap was estimated using the Perdew-Burke-Ernzerhof (PBE) and modi_ed BeckeJohnson potential, which con_rmed that as pressure increased, the band gap decreased in almost a linear manner.

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, chronoamperometry 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 (FeS$_2$) 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 (FeS$_2$) 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 (FeS$_2$), Nanoparticles, Molecular Dynamics

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**CO 17**

**Computational study of anatase TiO$_2$ nanotube as an anode material for lithium ion batteries**

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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:** TiO$_2$, DFTB+ potentials.

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**CO 18**

**First-principles studies of chromium line-ordered alloys in a molybdenum disulfide monolayer**

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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 (MoS$_2$) 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 MoS$_2$ system following the Vegard’s law. From density of states analysis, we found that the MoS$_2$ 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 MoS$_2$ monolayer are good candidates for nanotechnology devices.
**Keywords:** density functional theory, *ab-initio* simulation, electronic structure, two dimensional materials, molybdenum disulfide.

**CO 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-Saharan 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
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, Phosphorene, h-BN, SiC

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**CO 21**

**Catalysts for African Development and Advancement [CADA]**

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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(PO$_3$)$_2$. Preliminary SEMD simulations of possible catalysts for photocatalytic water splitting will also be presented.

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

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**CO 22**

**Li states on a C-H vacancy in graphene: 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$_{\text{CH}}$) in a graphene monolayer. The effects of a Li atom on the thermodynamic stability, structural, magnetic and electronic properties of a V$_{\text{CH}}$ defective graphene monolayer are explored, taking into account the effect of charge doping. We find that the Li ions enhance the thermodynamic stability of a V$_{\text{CH}}$ defective graphene monolayer. The partial density of states analysis suggests that the Li-V$_{\text{CH}}$ 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-VCH 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-VCH 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 VCH defective graphene 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 LaFeO$_3$(010) Surface for Use in Nickel-metal Hydride Batteries

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The ABO$_3$ perovskite lanthanum ferrite (LaFeO$_3$) is a technologically important electrode material for nickel–metal hydride batteries, energy storage and catalysis. However, the electrochemical hydrogen adsorption mechanism on LaFeO$_3$ 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 H$_2$ on the LaFeO$_3$(010) surface. We show from our calculated adsorption energies that the preferred site for H$_2$ 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. H$_2$ adsorption at the surface oxygen resulted in the formation of a water molecule, which leaves the surface to create an oxygen vacancy. The H$_2$ 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 LaFeO$_3$.

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

**CO 25**

**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 $\Phi$, 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 P$_4$), 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
CO 27

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
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 dye-sensitized 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
Presently used commercial lithium ion batteries (LIBs) consist of layer-type lithium cobalt oxide, spinel LiMn$_2$O$_4$ or LiFePO$_4$ as the cathode, graphite as the anode, and a non-aqueous Li$^+$ ion conducting solution or immobilized gel-polymer as an electrolyte$^1$. 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 SnO$_2$ and ternary oxides Nano-MCo$_2$O$_4$ (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.

**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, electroanalytical, 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
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 09

Funding for Tools for Materials Research at the National Science Foundation

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The complexity of modern materials research “is such that new advances in the field depend on strong support for large facilities, medium scale facilities, interdisciplinary research centers, and individual investigators who actually carry out the research.” We will provide an overview of the portfolio of Division of Material Research enabling access to instrumentation at all scale to materials researchers and educators at universities and colleges. These range from access to laboratory instrument to large scale facilities that are open to all on the basis of competitive proposal process.

EDO 10

Implementation of professional and academic development camp for Liberian women undergraduate engineers at the University of Liberia

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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 post-camp 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
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

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**EDO 12**

**Fostering an Entrepreneurial Mindset**

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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
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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
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.

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

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
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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)
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3School of curriculum and teacher education, University of Dodoma, Dodoma, Tanzania
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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-rich environment and videos demonstrating the taught
concepts, and simple classroom experiments. The methodology 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-Saharan 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.
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

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**EDO 21**

To achieve research excellence in Africa through networking and collaboration: Lessons learnt from the African Materials Science and Engineering Network

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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 landscape.

**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 ways 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
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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, commercialisation, entrepreneurship, skills, investment.

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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
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.
# POSTER PRESENTATIONS

## HEALTH

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| **HP 01** | **Inhibition of α-amylase by *Euclea crispa* phytochemicals: Implication for herbal management of diabetes mellitus type 2**  
Pamhidzai Dzomba and Tinevimbo Chidavayenzi  
Bindura University of Science Education, Faculty of Science, Chemistry Department  
P Bag 1020, Bindura, Zimbabwe  
Email: pdzomba@gmail.com |

Diabetes mellitus type 2 (DM 2) has become a global health concern with its current treatment regime limited by the side effects and mechanism of action. Thus the diseases has attracted much attention of the general public, researchers and pharmaceuticals companies. This study was designed to investigate the in-vitro alpha amylase inhibitory activity of phytochemicals extracted from the root barks of *Euclea crispa* as an alternative herbal therapy to DM 2. *Euclea crispa* is widely used to treat diabetes mellitus in folk role medicine. The phenolic acids and flavonoids were extracted by liquid-liquid extraction in ethanol. They were separated by analytical TLC followed by isolation by preparative TLC and further confirmed by FT-IR. Their inhibitory activity was established by measuring the absorbance of the starch iodine complex in a solution of starch, iodine, alpha-amylase and the phytochemicals. The inhibition was expressed as percentages and they ranged from 87% to 19% over a concentration range of 3-0.5 µg/ml with flavonoids exhibiting higher inhibitory activity than phenolic acids. The IC50 determined from the plot of concentration against percentage inhibition was found to be 1.0001µg/ml for flavonoids and 1.0065µg/ml for phenolic acids. The present results show that *Euclea crispa* phytochemicals are possible alternative herbal therapies for DM 2. Thus they can also be future health materials for developing lead compounds for DM 2 drugs. |

| **HP 02** | **Experimental analysis of low density poly ethylene effect on the mechanical properties of poly ethylene vinyl acetate for prosthetic and orthotic application**  
Yenealem Yilma  
Ethiopia biotechnology institute, Addis Ababa, Ethiopia  
Email: yenealemy@gmail.com |

In this comparative study, the effect of low density poly ethylene and ethylene vinyl acetate loading ratio by melt blending with additives and without additives on mechanical properties for prosthetic and orthotic application was analyzed. To carry out this thermoplastic materials such as low density poly ethylene (LDPE), Ethylene vinyl acetate (EVA), color pigment, calcium carbonate, titanium dioxide and black carbon have been used as raw material to produce the sample in sheet form and to achieve comfortable prosthetic and orthotic application. The method used were blending, molding, testing of produced materials. Increasing the content of EVA and decreasing content of LDPE had effect on compatibility, tensile strength and elongation at break vice versa. The blended composite with additives have no significant effect on molding and without additive have significant effect on molding due to molecular mobility which leads shrinkage. The maximum tensile strength reached to 10.5Mpa and minimum tensile strength reached 2.8Mpa and the maximum elongation at break reached 469.8% and minimum elongation at break 40.2%.The other result are in between of these ranges, which have better than existing one has maximum tensile strength of 2.3Mpa and elongation at break have 265%.The mean value of maximum tear load is 74.4N/mm and minimum tear load have 38.9N/mm which have better result than existing one has 10.5N/mm. Scanning electron microscope(SEM) test result showed that specimen with more filler and less content of EVA become poor in its morphology and compatibility. |

| **HP 03** | **Effect of precursor concentration on the size and shape of silver nanoparticles and their antimicrobial activity** |
Problems associated with the resistance of some microorganisms to antimicrobial agent is growing. The resistant microorganisms are a threat to human health because they are responsible for different diseases that are problematic to mammals. As part of the ongoing search for new antimicrobial agent that will have strong antibacterial activity against some resistant microorganism such as staphylococcus aureus, a diverse research is being conducted in different field such as medicinal plants and bio-nanotechnology. The current study focuses on the antibacterial and antifungal activity of silver nanoparticles prepared under different precursor concentrations. Silver nanoparticles were characterized using Uv-vis spectroscopy, Fourier Transform Infrared Spectroscopy (FT-IR), Transmission electron microscopy (TEM), X ray diffraction (XRD) and Photoluminescence (PL). TEM results showed that the particle size is directly proportional to the precursor concentration. A face-centred cubic crystalline structure of metallic silver was obtained from the XRD. The synthesized silver nanoparticle also showed satisfactory antifungal and antibacterial activity against Candida albicans, Cryptococcus neoformans, Staphylococcus aureus, Enterococcus faecalis, Klebsiella pneumonia and Pseudomonas aeruginosa. The MIC values obtained were between 0.20 and 6.25 mg/ml.

Drop casting method was used for the fabrication of modified electrode of sulphonated polyether ether ketone/zinc oxide (SPEEK/ZnO) nanocomposite on the gold electrode towards electrochemical oxidation of dopamine. The SPEEK/ZnO nanocomposite was characterized by using Fourier transform infrared (FT-IR), Uv-vis, the surface morphology were assessed by scanning electron microscopy (SEM) and elemental composition was characterized by using Electron dispersive spectroscopic (EDS). The electrocatalysis of dopamine was examined by suing cyclic voltammetry at gold electrode (Au) modified with SPEEK/ZnO nanocomposite in 0.1 M phosphate buffer solution PBS at pH 7. The result obtained at Au/SPEEK/ZnO modified electrode was compared with those obtained at the bare Au and Au/SPEEK nanocomposite modified electrodes. It was found that the zinc oxide nanoparticles increased the electroactivity of SPEEK for dopamine oxidation. For the quantitative analysis of dopamine (DA), the Au/SPEEK/ZnO electrode exhibited good linear properties in the concentration range from 5.4 x 10^{-14} to 1.9 x 10^{-14} µM with a sensitivity of 217.4 µA mM^{-1} cm^{-2} and a limit of detection of 0.85 nM. The modified Au/SPEEK/ZnO also gave a distinct separation peaks signal for dopamine and ascorbic in a mixture of both analytes. Also a satisfactory stability result was recorded for the modified electrode when stored at room temperature for several days and was successfully used to assay dopamine in real sample.
Nanosized particle of zinc oxide has gained much attention due to several applications which includes bacterial inhibition. Therefore, this work evaluates zinc oxide properties synthesised using reduction and bio-reduction processes and their corresponding inhibition potentials. The bio-reduction process was achieved using *Amaranthus spinosus* at 70°C while reduction process was initiated in the chemical process using sodium hydroxide. The synthesized nanoparticles were characterized for structural, optical and morphological properties using Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), UV-vis absorption spectroscopy, and Scanning Electron Microscopy (SEM). The antimicrobial activity of the synthesized nanoparticles was tested against *Pseudomonas aeruginosa*, *Salmonella typhi* and *Shigella dysenteriae*. The degree of susceptibility of ZnO nanoparticle was higher in bio-reduction process than chemically synthesized for selected microorganisms. A sustainable pathway for development of bio-antibiotic is presented.

Spices been a semi-perishable horticultural crops gets subjected to deterioration during storage, which ultimately leads to huge monetary loss and poses threat to national food security. Specific detection tools to detect this spoilage even before they are visible to the eye will be an asset in relieving these losses during post-harvest storage. In the context of this work, silver colloidal nanoparticle was synthesised using green method. *Elaesis guinesis*, *datura stramonium*, and *aloe-vera* were used as reducing and capping agent. The mixture of silver nitrate and plant extracts were heated for 30mins at 70°C and the colour was changed from light brown to dark brown showing reduction of silver. The reduction of silver was monitored using UV-Vis photospectrometer. X-ray diffraction technique (XRD), Scanning Electron Eicr oscopy (SEM) and Energy Dispersive X-ray Spectroscopy (EDX) were used to characterised the nanoparticles. The peak of the colloidal solution gotten using *elaeis, datura, and aloe-vera* as reducing agents was formed at 450nm, 380nm, and 350 nm respectively. This shows the bio reduction of Ag⁺ to Ag⁰. The visual changes during spoilage was monitored for 12 days, wherein, the dark brown colour of the silver colloidal solution change to light brown, pink and finally turned transparent. This present a sustainable pathway for post-harvest deterioration control of spices.
This research effort implemented a technique for resolving differential diagnosis in medical disease diagnosis expert systems. This was achieved by collecting additional information from users during diagnosis which help to correctly decide which new rule will be asserted to the working memory before feedback can be deduced after proving that a user is suffering from a particular disease by confirming all the symptoms. Our approach correctly resolves differential diagnosis by ruling out similar diseases which match user disease symptoms and enhances the general accuracy of the expert system due to sufficient user information made usable to the system. This work presents a general solution to most significant problem of differential diagnosis which is neither restricted to a particular disease nor medical domain as compared to the work of other researchers where techniques to resolve differential diagnosis were restricted to a particular disease type. The system can be further optimized by providing the probability value when a goal is achieved as well as medical prescription after diagnosis is completed.

<table>
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<th>HP 08</th>
<th>Antioxidant Activity Levels of Phenolic and Flavonoid Contents in Methanol Extract and Solvent Fractions of <em>Desmodium ramosissimum</em></th>
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<td>V.N. Ogugua¹, P.E. Joshua², M.O. Agbo², U.S. Ezealigo³</td>
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<td>¹University of Nigeria (Department of Biochemistry, Nsukka, Nigeria)</td>
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<td>²University of Nigeria (Department of Pharmaceutical Science, Nsukka, Nigeria)</td>
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<td>³African University of Science and Technology (Department of Materials Science and Engineering, Abuja, Nigeria).</td>
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<td>Email: <a href="mailto:uezealigo@aust.edu.ng">uezealigo@aust.edu.ng</a></td>
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The present study was designed to estimate the total phenolic and flavonoid contents. It also evaluates the *in vitro* antioxidant activities of both the methanol extract and the various solvent fractions of the whole plant, *Desmodium ramosissimum*. The quantitative phytochemical analyses of the total phenolic content (TPC) and total flavonoid content (TFC) were carried out spectrophotometrically using Folin-Ciocalteu phenol reagent and aluminum chloride method respectively. The phytochemical screening revealed the presence of various bioactive components such as phenolics, flavonoids and tannins. Ethyl acetate fraction followed by *n*-butanol fraction exhibited higher total antioxidant activity among other solvents. The relationship between the antioxidant content using various models also revealed that (TPC) exhibited a strong correlation with ferric ion reducing potential (FIRP) and total antioxidant capacity (TAC) with R² values of 0.995 and 0.980, respectively; while a weak relationship with 1,1-diphenyl-2-picrylhydrazyl (DPPH) radical with R² value of 0.877 was observed. However, aqueous fraction showed a strong relationship between DPPH and its concentration compared to other fractions. In addition to these, several solvent fractions possess unique chemical constituent of plant with various antioxidant capacity. Free radicals were scavenged by the extract and solvent fractions in a concentration-dependent manner within the range of the given concentrations (25-1000 mg/ml) in all models. This is an indication that the methanol extract and solvent fractions of *Desmodium ramosissimum* G. Don contains phenolics, flavonoids and tannins which exhibited antioxidant properties. The presence of these flavonoid and phenolic compounds contribute to the antioxidant properties observed in the whole plant.

<table>
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<th>HP 09</th>
<th>Optimization of extraction of phenolics from Rose geranium leaf using RSM and evaluation of kinetics model of antioxidant activity against DPPH radicals</th>
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<td>Makanyane, M.D¹, Mtnzni, F.M², Ssemakalu, C³</td>
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<td>¹Department of chemistry, Private bag x021, Vaal University of technology</td>
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Polyphenols are multifunctional secondary metabolites in plants. However, due to less information available concerning the statistical actual yield, optimal extraction method and pharmacological activity with regards nonvolatile compounds from *Rose geranium* leaves. Hence, response surface methodology (RSM) was used to optimize extraction parameters. The effects of the independent variables under study were speed of agitation (rpm), volume of methanol solvent (mL), time of extraction (hrs.) and mass of plant material (grams). The antioxidant activity was assessed with DPPH assay, the kinetics of DPPH radicals against methanol crude extracts were characterized with UV/VIS spectrometer. A polynomial quadratic model produced satisfactory fitting of experimental data, for % yield ($R^2 = 0.9943$, $P<0.0001$), total phenols ($R^2 = 0.9621$, $P<0.0001$). The best combination was obtained at (3g, 100 mL, 100 rpm, and 24hrs) for % yield, total phenols at (0.522g, 199.499 rpm, 20.572hrs), and 73.263 mL. The yield of *Rose geranium* methanol extract reached 333.412 mg, total phenols (61.25±0.073 mg GAE/g) under the above conditions. IC$_{50}$ values for DPPH assay percentage inhibition was quercetin (0.101±0.00106 µg/mL)> garlic acid (0.224±0.00212 µg/mL)> ascorbic acid (0.468±0.000884 µg/mL)> methanol extract (0.742±0.00279 µg/mL). The RSM was successfully used for optimizations, the obtained data can further be used for biological applications.

**Quantum Dots-Electro-sensitised Phenotype Sensor for Breast Cancer Drug**

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Tamoxifen is the most prescribed breast cancer drug, as it is used for the treatment of all stages of breast cancer disease. However, variations in the responses of patients to treatment with the drug is of great concern to clinicians, due to the possibility of the occurrence of drug toxicity or resistivity. Thus, there is need for the development of cost effective diagnostic protocols suitable for monitoring the rate of metabolism of the drug at point-of-care in order to ensure adequate personalised therapy. This study involved the development of next generation phenotype-based diagnostic nanobiosensors (b-cancernanosens) for determining a breast cancer patient’s response profile (poor, moderate or ultra-rapid metaboliser) for tamoxifen. The sensor consists of cytochrome P450-3A4 (CYP3A4) enzyme and thioglycolic acid capped palladium telluride quantum dots (TGA-PdTeQDs) bio-reactor on a gold sensor chip modified with cystamine (Cyst). The TGA-PdTeQDs analyses by high resolution transmission electron microscope (HR-TEM) and small angle X-ray scattering spectroscopy (SAXS) revealed that the quantum dots have average diameters of 2-5 nm. The b-cancernanosens (i.e. CYP3A4|TGA-PdTeQDs|Cyst|Au biosensor system) gave a limit of detection (LOD) value of 9.52×10⁻⁵ ng/mL, tamoxifen at a square wave voltammetry (SWV) potential of 0.28 V. The LOD value obtained was lower than tamoxifen’s maximum steady state plasma concentration ($C_{max}$ 40 ng/mL, normally obtained 5 h after drug administration). This indicates that the sensing device, in principle, would be suitable for real time monitoring the breast cancer drug at point-of-care.

**Synthesis of folate-conjugated palladium nanoparticles**

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Nanomaterials have open doors to different application because of their unique properties such as surface compared to bulk material. The nanoparticles have been used as potential drug delivery system owing to the ease of tailoring the surface with substituents which contributes to high selectivity and biocompatible. Folate is important in cell growth and division. The folate receptors
are over expressed in cancer cells as they need more of the folate to produce more cancer cells. The use of folate has been applied in gold nanoparticles for cancer cell imaging and killing cancer cells with less damage to normal cells. The study was carried out via two routes; firstly the synthesis of palladium nanoparticles capped with 4-aminothiophenol and 2-aminobenzethiol (2-Aet) prior to the folate being introduced. The 4-Atp-PdNPs were characterized by Fourier Transform Infrared spectroscopy (FTIR), and UV-Vis spectroscopy to study the formation of the target product (4-Atp-PdNPs). The same was done to the 2-Aet-PdNPs product. The palladium nanoparticles were synthesized in the presence of the capping agents. The optical properties of the product formed was studied using UV-Vis spectroscopy and the size and shape as well as the chemistry of the nanoparticles were obtained from the Transmission Electron Microscope (TEM), X-Ray Photoelectron Spectroscopy (XPS), Fourier-Transform Infrared spectroscopy (FTIR), Photoluminescence (PL). These results will be presented and discussed.

**HP 12**  
Composite Poly(3-4-propylenedioxythiophene)-Gold Nanoparticles (PProDOT-AuNPs) for the Development of Ultrasensitive DNA Atpasensor for Interferon Gamma Tuberculosis Biomarker

Unathi Sidwaba¹, Tesfaye Waryo¹, Phillipa Randall², Keertan Dheda², Priscilla Baker³, Emmanuel Iwuoha³

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Although tuberculosis (TB) is a curable disease, its total control and eradication remains a challenge due to emergence of drug-resistant strains, high default rates (incomplete treatment), the dormant behaviour of the TB-causing bacteria and co-infection with other disease such as diabetes and human immunodeficiency virus (HIV) which complicate both diagnosis and treatment. Hence, early diagnosis of the disease, possible through detection of the bacteria causing the disease and biomarkers is of pivotal importance towards control of the TB epidemic. Up to date, electrochemical assays employing nanomaterials such as gold nanoparticles, disease-prompting agents such as interferon gamma (IFN-γ) and target-specific agents like aptamers have shown to circumvent the low sensitivity and poor selectivity issues associated with available diagnostic methods. Herein, an ultrasensitive aptasensor system was fabricated by assembling a DNA aptamer specific to IFN-γ onto a novel poly(3-4-propylendioxythiophene)-gold nanoparticles (PProDOT-AuNPs) nanocomposite. Electrochemical impedance spectroscopy (EIS) signal changes induced by PProDOT-AuNPs/aptamer and aptamer/IFN-γ binding interactions were monitored during fabrication and detection of IFN-γ, respectively. Finally, the performance of the aptasensor was tested towards detection of IFN-γ in spiked pleural fluid samples. The aptasensor system exhibited a low detection limit of 2.2 pg/mL and a linear detection range with a minimum value of 0.4 pg/mL and a maximum value of 1.4 pg/mL. Ability of the aptasensor system to detect IFN-γ in pleural fluid samples and to discriminate IFN-γ from other species such as LAM highlights potential application of the system towards detection of TB in clinical samples.

**HP 13**  
Quantum dots amplified DNA-Aptasensor for TB biomarker detection

Kaylin Januarie, Lindsay Wilson, Emmanuel Iwuoha

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Tuberculosis (TB) is one of the major infectious diseases that affect the health of people all over the world. Various tests have been used to diagnose tuberculosis infected patients but some of these tests are unreliable as they sometimes give false positive results. Studies have shown that TB related cytokines signalling proteins, such as interferon-gamma (IFN-γ) can serve as biomarkers for the diagnosis of the disease [¹]. IFN-γ related test for TB currently in use are antibody-based immunosensing techniques which are very expensive and time consuming. It is thus vital that an
alternative detection method for IFN-γ be developed. This presentation deals with the development of a fast, simple and sensitive QDs-based electrochemical DNA aptamer biosensor (aptasensor) for the detection of IFN-γ. The aptasensor consists of indium tellurium selenide (InTeSe) quantum dots capped with L-cysteine to produce a DNA aptamer sequence for IFN-γ on a gold electrode. The optical properties of the QDs were characterized by UV-vis and fluorescence (FL) spectrometry which gave an absorbance band at 291 nm and emission band at 320 nm. The structure of the QDs was verified by Fourier transform infrared spectroscopy (FTIR) and high resolution transmission electron microscopy (HRTEM). HRTEM revealed that the QDs consist of 7 nm particles. The electrochemical response parameters of the QDs aptasensor for IFN-γ were studied by cyclic voltammetry (CV), square wave voltammetry (SWV) and electrochemical impedance spectroscopy (EIS). For EIS the aptasensor had a sensitivity of $2.2 \times 10^5 \text{ Q/(pg/mL)}$ and a detection limit of 3 pg/mL.

### HP 14
**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 nanoparticle 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.

### HP 15
**Impedimetric phase angle immunosensing of LAM TB biomarker on sulfonated polyaniline screen printed carbon electrode**

Lindsay Wilson, Tesfaye Waryo, Christopher Sunday, Phillipa Randall, Keertan Dheda, Emmanuel Iwuoha

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2. Lung Infection and Immunity Unit, Department of Medicine, University of Cape Town, Cape Town, Republic of South Africa

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The diagnosis of tuberculosis (TB) through the detection of TB biomarkers, such as lipoarabinomannan (LAM), in bodily fluids of infected individuals can significantly reduce mortality rates from this disease. Currently, the GeneXpert MTB/RIF and Alere Determine TB LAM Ag test have become the diagnostic gold standards, but suffers from high costs (GeneXpert) and low sensitivity (Alere test). The two tests focus on the detection of LAM in urine. The work being reported is focused on the development of a LAM immunosensor on poly(4-styrene sulfonic acid)-
doped polyaniline (PANI-PSSA) film which is electrodeposited on screen printed carbon electrodes (SPCE). The SPCE modification steps and the interactions between the antiLAM antibody and LAM antigen were monitored by the shifts in the phase angle signals of the Bode formulation of the electrochemical impedance spectroscopy (EIS). The phase angle signal shifts were measured at a single frequency, and the magnitude of the signal is related to the interactions associated with the SPCE modification steps and those of the antiLAM and LAM binding. The EIS phase angle-based immunosensor, produced a linear detection range of 100 - 400 pg/mL LAM, a limit of detection of 27 pg/mL LAM and a sensitivity of 0.0478°/(pg/mL LAM). The immunosensor also allowed for qualitative detection of LAM in spiked urine and clinical samples.

<table>
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<th>HP 16</th>
<th>Extraction and Characterization of Chitosan from Black Soldier fly (<em>Hermetia illucens</em>)</th>
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<tr>
<td>Monushia N. Zimri¹, Cosmas C. Uche¹, Leslie Petrik¹, Roland Missengue¹, Yuri Kochnev²</td>
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<tr>
<td>¹University of the Western Cape (Chemistry, Cape Town (Bellville), South Africa)</td>
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<td>²Joint Institute for Nuclear Research (Flerov Laboratory of Nuclear Reactions, Dubna, Russia)</td>
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<td>Email: <a href="mailto:3140545@myuwc.ac.za">3140545@myuwc.ac.za</a></td>
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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 ($T_{\text{max}}$) 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 $T_{\text{max}}$ 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.

<table>
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<th>HP 17</th>
<th>Effect of Sintering Time on Mechanical Properties of Porous Ti-6Al-4V Implant</th>
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<tbody>
<tr>
<td>A.A. Azeez¹, ², Y. Danuyo³, J. D Obayemi³, W.O. Soboyejo⁴, ⁴</td>
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<tr>
<td>¹ Department of Materials Science and Engineering, African University of Science and Technology, Abuja, Nigeria.</td>
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<td>² Department of Physics, Nile University of Nigeria, Abuja, Nigeria.</td>
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<td>³ Department of Materials Science and Engineering, Kwara State University, Malete Kwara State, Nigeria.</td>
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<tr>
<td>⁴ Department of Mechanical Engineering, Worcester Polytechnic Institute, 100 Institute Rd, Worcester, MA 01609, USA</td>
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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.

**HP 18**

**Prodigiosin Induced Apoptosis and the Cytoskeletal Changes on Breast Cancer Cell Line Mda-Mb-231.**

S. O. Dozie-Nwachukwu\(^1,2,4\), J. D. Obayemi\(^4\), A. A. Salifu\(^4\), O. S. Odusanya\(^1,2\), A. Nzihou\(^3\) and W. O. Soboyejo\(^1,4\)

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Prodigiosin, a tripyrrole red pigment, was extracted from *Serratia marcescens*. Its apoptotic effect was tested on the human breast cancer cell line, MDA-MB-231. The cytotoxicity of prodigiosin was also tested using the Alamar blue assay, which was found to be up to 80% effective. The changes in the actin microfilament architecture and the cytoskeletal structure were elucidated with optical, scanning electron and confocal microscopy. The cell viability was also shown to decrease with increasing drug diffusion. The morphological analysis of prodigiosin-treated cells revealed that prodigiosin induces cell shrinkage, chromatin condensation, the reorganization of the actin microfilament architecture, and the detachment of cells from the substrate. These implications of the results are discussed for the treatment of breast cancer.

**HP 19**

**Ru(li/iiii) Complexes of Polypyridyl Ligands with Anti-Bacterial Properties.**

Lebogang G. Julius\(^1\), Daphne Mapolelo\(^1\), Florence Naretsile\(^1\), James T.P. Matshwele\(^2\), Pearl Matshameko\(^3\), Melvin Leteane\(^3\) And David Nkwe\(^4\)

\(^1\)University of Botswana (Department of Chemistry, Gaborone, Botswana)
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Ruthenium-based complexes have become the interest of drug development research due to their properties that are well suited towards pharmaceutical applications. Herein we report the synthesis and characterization of a bidentate pyridyl ligand = [(2-PC)], and octahedral amino pyridyl based ruthenium complexes being [Ru(BBE)(2-PC)(Cl)]\(_2\) and [Ru(DPA)(2-PC)(Cl)]\(_2\). The ruthenium complexes were synthesized from Li[Ru(BBE)(Cl)]\(_4\) and Li[Ru(DPA)(Cl)]\(_4\) intermediate complexes respectively. Spectroscopic characterization of the synthesized complexes was done by FTIR, GC/MS and UV-vis spectroscopy. The synthesized complexes were then tested against series of both gram-positive and gram-negative bacteria strains being *E. coli*, *P. aeruginosa*, *K. pneumoniae*, *Multi-Drug resistant-K. pneumoniae*, *S. aureus* and *Methicillin-resistant Staphylococcus aureus (MRSA)*. Bacterial strains proved inhibited growth to the complexes [Ru(BBE)(2-PC)(Cl)]\(_2\) and [Ru(DPA)(2-PC)(Cl)]\(_2\) and intermediate complexes [Li[Ru(BBE)(Cl)]\(_4\)] and [Li[Ru(DPA)(Cl)]\(_4\)] and reported in this work are the Minimum Inhibition Concentrations (MIC) as determined by the Kirby disc diffusion assay.
### Determination of Metal (Micronutrients) Content from Non-Edible Plant Parts of Morula (Sclerocarya Birrea), Mango (Magnifera Indica L.) and Moringa Oleifera Seed Pods

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Indigenous fruits/plants are important as they play a vital role in the lives of human beings, they provide food security, health and nutrition, and economic welfare of rural communities in the developing world, of recent there has been a grown interest in the utilization of what has become to be known as multipurpose plants. The waste that result from some of these fruits can be recycled as stock feed or food supplements for human consumption, hard materials used as adsorbents for removing contaminants from wastewaters and the plant parts of these trees can be used for medicinal purposes which is most widely used locally. Some of these indigenous plants mango (Magnifera indica L.), moringa oleifera and morula (Sclerocarya birrea), which carry mineral elements among these elements includes (Na), (Mn), (Fe), (Zn), (Ca) and (Cu). These elements both macro and micro elements play an essential role in the human body mineral elements are essential for life growth and development. So, we herein report the metal content (micro-nutrients) from non-edible plants of moringa oleifere seed pods, morula (Sclerocarya birrea) and mango (Magnifera indica L.) using Flame atomic absorption spectroscopy, also studied the effect of storage on morula fruit peels and juice and further studied moringa oleifera by characterization using Fourier transformer infra-red (FTIR) and analysing the efficiency of metal extraction from moringa oleifera seed pods was studied as well using boiling water and also after acidification (adding acidified lemon juice).

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### Metal Ligand Design for Diagnosis and Therapy

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Metal ions play a vast number of widely differing biological processes/systems. Metal ions that are essential in human life include calcium, magnesium, manganese, iron, cobalt, copper and zinc. Greater percentage of these ions is bound to proteins and only a small fraction is bound to low molecular mass (l.m.m.) compounds mainly amino acids. Of particular interest is concentration of l.m.m. complexes of copper which rises in patients with rheumatoid arthritis. There is great effort in development of radiopharmaceuticals for the diagnosis and therapy of the metastatic bone cancer. This effort relies heavily on the use of radiolabelled receptor ligands. Because of high specificity and selectivity, the radiolabelled receptor ligands offer advantages over traditional perfusion radiotracers. This study is based on the design and synthesis of ligands that would (a) effectively mobilise trivalent lanthanides (e.g. samarium, lutetium) to the site of cancer for diagnosis and treatment and (b) effectively mobilise copper complex to the synovial site during rheumatoid arthritis for treatment of inflammation. Chemical speciation for metal ligand interaction will be determined by pH glass electrode potentiometry at 25 °C and ionic strength 0.15 mol dm⁻³. ESTA library of programs will be used to evaluate the stability constants. UV-visible spectrophotometry will be used to elucidate structures of the different species in solution. Bio-modelling is performed by blood plasma model that incorporates formation constants obtained from potentiometric results. Results will be discussed and presented.
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| **EP 01** | **Cold welding of organic light emitting diode: Interfacial and contact models**  
J. Asare,1,2 S. A. Adeniji,3 O. K. Oyewole,1,2,4 B. Agyei-Tuffour,3 J. Du,5,6,7 E. Arthur,3,4 A. A. Fashina,1  
M. G. Zebaze Kana,1,4 And W. O. Soboyejo1,6,7  
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This paper presents the results of an analytical and computational study of the contacts and interfacial fracture associated with the cold welding of Organic Light Emitting diodes (OLEDs). The effects of impurities (within the possible interfaces) are explored for contacts and interfacial fracture between layers that are relevant to model OLEDs. The models are used to study the effects of adhesion, pressure, thin film layer thickness and dust particle modulus (between the contacting surfaces) on contact profiles around impurities between cold-welded thin films. The lift-off stage of thin films (during cold welding) is then modeled as an interfacial fracture process. A combination of adhesion and interfacial fracture theories is used to provide new insights for the design of improved contact and interfacial separation during cold welding. The implications of the results are discussed for the design and fabrication of cold welded OLED structures. |
| **EP 02** | **Microstructure evolution and thermoelectric properties of Te-poor and Te-rich (Bi,Sb)₂Te₃ prepared via solidification**  
Olu Emmanuel Femi1, N. Ravishankar2, K. Chattopadhyay2  
1 Jimma University, Department of Material Engineering, Jimma Institute of Technology, Jimma-378 Ethiopia  
2 Indian Institute of Science, Materials Research Centre, Bangalore-12, India  
3 Indian Institute of Science, Department of Materials Engineering, Bangalore-12, India  
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This work comprehensively examine, the microstructures and thermoelectric properties of Te-rich and Te-poor (Bi,Sb)₂Te₃ alloys. We demonstrated that tuning the composition of ternary Bi-Sb-Te type alloys enables us to synthesize different microstructures containing a primary solid solution of (Bi,Sb)₂Te₃ with varying amounts of Te solid solution or a (Bi,Sb)Te compound. Te exists as a constituent of the multilayer domain while (Bi,Sb)Te appears in the thin intercellular regions of the (Bi,Sb)₂Te₃ dendritic cells. The presence of Te imparts an n-type behavior to the composite while the (Bi,Sb)₂Te₃ with a small amount of (Bi,Sb)Te exhibit p-type properties. A maximum ZT value of ≈ 0.4 at 425 K was achieved, opening up the possibility of using these alloys for thermoelectric device applications. |
| **EP 03** | **Effect Of Transition Metal Dopants On The Properties On Copper (I) Iodide Thin Films Grown On a Glass Substrate By SILAR Method.** |
Aluminum (Al), Lead (Pb) and Zinc (Zn) were used as dopants for cuprous iodide (CuI) films at room temperature deposited by successive ionic layer adsorption and reaction (SILAR) method. The effect of these dopants on the surface morphology, optical properties, structural properties, photoluminescence properties and electrochemical properties was studied. The XRD diffractograph showed a face-centered cubic crystal structure with high peak at (111) orientation. The Williamson and Hall (W-H) analysis was used to determine the crystallite size and lattice strain of the deposited thin films.

A high optical transmittance was observed for all doped films, with photoluminescence in the early visible spectrum (400-440 nm). Also, high optical conductivity value was observed for the dopants as the photon energy increases except for the Pb-doped film. The energy band gap for the material varied from 1.90 to 2.80 eV, the Aluminum doped films gave the maximum specific capacitance of 116 Fg$^{-1}$ at 2 mV/s scan rate.

EP 04 Extraction of oil from Datura Stramonium Seeds as Potential Feed-Stock for Bio-Diesel Production

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Energy demand is increasing due to the expanding population growth in Botswana and the world at large. It has become apparent that biodiesel is destined to make a substantial contribution to the future energy demands of the domestic and industrial economies. Non-edible plant oils which are known as the second generation feed stocks can be considered as promising substitutions for traditional edible food crops for the production of biodiesel. The use of non-edible plant oils is very significant because of the tremendous demand for edible oils as food source. Moreover, edible oils’ feedstock costs are far expensive to be used as fuel. Therefore, production of biodiesel from non-edible oils is an effective way to overcome all the associated problems with edible oils. However, the potential of converting of non-edible oil into biodiesel must be well examined as the physical and chemical properties might differ from that of edible oils, hence the need for this research where oil was extracted from the Datura stramonium seeds and analysed.

EP 05 Hydrogen Evolution Reactions of Conducting Polymer-Metal Organic Framework Nanocomposites

Kabelo E. Ramohlola$^{a}$, Siyabonga B. Mduli$^{8}$, Milua MasiKini$^{8}$, Mpitloane J. Hato$^{4}$, Kerileng M. Molapo$^{9}$, Emmanuel I. Iwuoha$^{8}$, Kwen D. Modibane$^{**A}$

$^a$ Department of Chemistry, University of Limpopo,
The development of highly efficient electrocatalysts for hydrogen evolution reaction is a fundamental undertaking of the hydrogen economy. Herein, we investigated the electrocatalytic performance of conducting polymer (polyaniline, poly (3-aminobenzoic acid)/metal organic framework (HKUST-1) nanocomposites for hydrogen evolution reactions. The results show that the synthesized nanocomposites exhibit the best electrocatalytic efficiency at lower overpotential and the Tafel analysis (transfer coefficient (α) and Tafel slope (β)) suggests that the rate-determining step is the Volmer (electrochemical discharge) coupled with either Tafel (chemical desorption) or Heyrovsky (electrochemical desorption) reactions.

Scheme 1: Synthesis of poly(3-amiobenzoic acid) doped with metal organic framework nanocomposite through in situ oxidation polymerization of 3-aminobenzoic monomer in the presence of MOF.

EP 06 Optical properties of PZN-PT nanoparticles thin layer on ITO glass for photovoltaic application
Remi Ndioukane¹, Diouma Kobor¹, Laurence Motte², Jeanne Solard³
¹University Assane Seck of Ziguinchor, Laboratoire de Chimie et de Physique des Matériaux (LCPM), Ziguinchor, Sénégal
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The past years witnessed a revolution in optoelectronic research with the discovery of the organic-inorganic lead-halide perovskite family. These solution-processable perovskites are fast becoming the most promising materials for the next generation of solar cells, achieving efficiencies above 22% due to the outstanding optoelectronic properties of perovskites such as methylammonium lead iodide. Despite this breakthrough, hybrid lead-halide perovskites are known to degrade due to moisture and heat, upon prolonged exposure to light and are prone to ion or halide vacancy migration, leading to unstable operation of photovoltaic devices. To overcome such difficulties, we oriented our research to inorganic PZN-PT perovskite materials with excellent and stable properties compared to the organic-perovskite ones. However, despite their excellent properties, one of the greatest difficulties to integrate widely such materials in electronic devices is to achieve them in thin films form because of their incongruent melting property. In this work, undoped and Mn doped PZN-4.5PT nanoparticles were dispersed in biopolymer and in mixte biopolymer + pentacene as active layer and deposited by spin coating on ITO glasses. Morphological, optical and electrical properties of these layers were investigated. SEM images show the superposition of different deposited layers ITO/TiO2/PZN-PT-mp-biopolymer on glass substrate with thicknesses of 1.600 µm, 1.505 µm and 1.765 µm respectively. The absorbance value in UV visible of such devices increases
from 75 % to 99 % while the transparency of ITO glasses diminishes from more than 80 % to 2 %
showing the potential application of such materials in solar cells.

**EP 07**

**Nano-Rod-Like Na\(_{0.44}\)MnO\(_2\) as Cathode Material for Sodium Ion Battery**

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Na\(_{0.44}\)MnO\(_2\) was synthesized by solid state method using Na\(_2\)CO\(_3\) and MnCO\(_3\). The XRD pattern indicated that it could be indexed as orthorhombic structured Na\(_{0.44}\)MnO\(_2\) with no impurities present. The TEM of the Na\(_{0.44}\)MnO\(_2\) shows that the material is rod-like with average length and width of 1-2 µm and 0.2-0.8 µm respectively while the EDS show the Na, Mn and O at the appropriate energy levels. The SEM confirms that the material is rod-like with uneven length and size while the NMR indicates the three peaks corresponding to three Na\(^+\) sites in the structure. The electrochemical properties were investigated in Swagelok-like cells using cyclic voltammetry, galvanostatic testing, and electrochemical impedance spectroscopy in various aqueous electrolytes such Na\(_2\)SO\(_4\), NaNO\(_3\), and NaClO\(_4\). Moderate capacities were obtained with appreciable coulombic efficiency.

**EP 08**

**Effects of Phosphoric acid electrolyte concentration and voltage on nanoporous anodic aluminium oxide films by one-step anodization**

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Nanoporous Aluminium (III) oxide was fabricated and characterized to determine its suitability as an antireflection coating. Aluminium (III) oxides were obtained using an anodization process with Phosphoric acid (H\(_3\)PO\(_4\)) as an electrolyte. Anodization voltage and electrolyte concentration were varied. Semi-ordered nanotubes were observed using a Scanning Electron Microscope. Porosity, pore diameter and interpore distance were obtained and were found to increase with an increase in anodization voltage. However, while the pore diameter and porosity increased with an increase in electrolyte concentration, the interpore distance was found to decrease. Reflectance curves showed a wide range of low reflectance in the visible light region.

**EP 09**

**Structural and electrochemical behaviour of platinum based binary nanomaterials (PtIr, PtRu, and PtTe) for electrocatalysis of ammonia for hydrogen production in fuel cell application**

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The electrocatalysts capped with polyvinylpyrrolidone (PVP) were highly specific and selective. The electrocatalysts were poly-orientate nanomaterials and platinum (Pt) face-centred-cubic crystal structure as revealed by X-ray diffraction. Fourier transform infrared spectroscopy (FTIR) showed the most striking evidence that the Pt is PVP stabilized due to the formation of coordinate bond between the nitrogen atom of the PVP and the metallic ions. Morphological characterization by
high resolution scanning electron microscope (HRSEM) and High resolution transmission electron microscopy (HRTEM) with particle size of 2-5 nm sized nanoparticles. The electro-oxidation of ammonia on platinum electrode drop coated with binary nanoalloys was systematically studied in alkaline solution of potassium hydroxide (KOH) by cyclic voltammetry (CV), square wave voltammetry (SWV) and electrochemical impedance spectroscopy (EIS). CV and SWV showed in terms of minimising the ammonia oxidation overpotential, electrocatalysts were ranked accordingly; PtTe > PtIr > PtRu. Maximising the exchange current density, were ranked PtTe > PtRu > PtIr respectively. The results were further interrogated with EIS which revealed in terms of minimising charge transfer resistance ($R_{ct}$) of nanomaterials were ranked as PtRu; $R_{ct} = 9.1004 \Omega$ > PtIr; $1.7707 \times 10^5 \Omega$ > PtTe; $4.8323 \times 10^{14} \Omega$ and $3.0507 \times 10^{12} \Omega$.

EP 10

**Conversion of Carbonized Biomass into Slurry Fuel for Electricity Generation**

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Biochar Slurry fuels which is a mixture of fine char particles in a liquid medium with some amount of additives has been proven to power compression ignition engines and capable of serving as a low carbon alternative to diesel fuel. However, no proven ratio has produced biochar slurry with sufficient energy density and suitable viscosity to foster commercial production or adaptation. Literature has described several particle loading concentration, but all have produced slurry with non-Newtonian and thixotropic behavior with shear-thinning properties that caused particle settling during storage, cavitation during fuel pumping through pipes, poor atomization and exorbitant wear of engine parts. This research is investigating optimization of biochar particle properties including particle size, volume fraction, participle size distribution, particles shape and zeta particle and applying multimodal system to improve volumetric energy density and viscosity. This method provide a superior way of developing an optimum blend ratios for a minimum viscosity against which a similar project can be piloted. Series of experiment on each of the five parameters is undergoing to match the corresponding properties that yield optimum values of viscosity and energy density. This approach is expected to be cheaper and simpler than the conventional route of transesterification to biodiesel since biomass from either forest or agricultural wastes readily available in most sub Saharan Africa.

EP 11

**Application of Natural Fibre Reinforced Composite for Satellite Antenna Dish Reflector Design.**

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The deployment of Satellite Communications in today’s broadband telecommunications cannot be over-emphasized. One major segment that plays a major role is the parabolic antenna dish reflector which is a part of the antenna system, a very robust telecommunication system can be degraded by the antenna system, hence the need for this research. Composite are basically a combinations of two or more materials, the reinforced phase in form of fibres or particles which are embedded in the other material known as the matrix phase, when this is achieved, we get the desired mechanical properties. The aim of this research is to use an indigenous technology to build an effective parabolic antenna dish reflector in quest for lighter components at reduced cost. Also, the use of natural fibre over the conventional metals will help to reduce cost and weight of these systems and further boost local contents, hence the need for this research.

EP 12

**Enhanced Performance of Antimony Sulphide Mesoscopic Solar Cells by Employing Nb:TiO2 Compact Layer**

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Antimony Sulphide has recently had much attention as a promising absorber material for photovoltaic devices and further studies are now focusing on optimization of the devices to improve their performance. A compact layer of TiO$_2$ is normally used in Mesoscopic and Extremely Thin Absorber solar cells to block holes from reaching the transparent conducting oxide electrode. Doping of this layer with transition metals and nitrogen has an impact in its electronic properties which influences the device performance. This work reports preliminary results on the enhancement of charge transport in Mesoscopic Antimony Sulphide solar cells with TiO$_2$ compact layer by doping with Niobium which led to solar cells with improved fill factor and power conversion efficiency (PCE) of 1.7% from 1.3% for devices using pristine TiO$_2$ compact layer. The enhancement of the device performance is attributed to charge compensation achieved by formation of Ti vacancies which leads to a decrease in selective contact resistance and an increase in charge recombination resistance as expected from the analysis of the impedance spectroscopy measurements.

**EP 13**

**Synthesis and modification of mesoporous TiO$_2$ nanomaterials using Gum Arabic as templating agent, and subsequent fluorine doping.**  
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Mesoporous TiO$_2$ was prepared by developing a sol-gel method using Gum Arabic as templating agent, Trifluoroacetic acid (TFA) as fluorine precursor for doping, and Titanium Methoxide (Ti(OCH$_3$)$_4$) as titanium precursor respectively. The purpose of this study was to elucidate the effect of surfactant and dopant on the pore size, specific surface area, band gap and structure of mesoporous TiO$_2$ by sol-gel method. The resulting materials were characterized with X-ray diffraction (XRD), Brunauer-Emmet-Teller (BET), Diffuse Reflectance Spectroscopy (DRS), Scanning Electron Microscopy (SEM) and Fourier Transform Infrared (FTIR) techniques. The XRD analysis of synthesized mesoporous powder, showed the formation of rutile phase as well as anatase in such a manner that the latter constituted a very small percentage of the titania. Moreover, the rutile’s phase content increases with the increase of the quantity of the fluorine precursor in the starting solution. The doped TiO$_2$ showed a red shift absorption in UV-vis region which was attributed to the increased content of rutile phase in the resulting material.

**EP 14**

**Optimization of Aqueous Electrolytes for electrochemical Double Layer Supercapacitors Application**  
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There is need for efficient energy storage to meet the world continuous demand for sustainable energy. The electrical energy storage devices are conventional capacitors, Electrochemical supercapacitor, batteries and fuel cells. The electrode materials play important role in improving the efficiency of energy storage system such as batteries and electrochemical supercapacitors. The electrochemical supercapacitors have power densities greater than those of batteries, energy densities greater than those of conventional capacitors and also maintain high cyclic life. Despite these advantages, electrochemical supercapacitors do not offer sufficient energy densities to
compared with the batteries and fuel cells. Therefore, there is need for research to improve the energy densities of electrochemical supercapacitor without compromising on their power densities. Carbon soot are potential carbon materials for fabrication of electrode for supercapacitor because they are cheap, abundant and readily available. Thus, we explored carbon soot as a potential electrode material for supercapacitors and also optimized different electrolytes for enhancement of electrochemical performance of the soot in order to improve the energy density of electrolytic double layer supercapacitor.

### EP 15

**Synthesis of KF/Cattle bone-Fe3O4 catalyst for single stage transesterification of high FFA oil**

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Single stage transesterification of oil with FFA of above 1 %w/w using cattle bone impregnated with potassium fluoride as catalyst for the reaction was the area of study. The experiment was done in two phases, first was the catalyst synthesis and the second is reaction optimization. Central composite design (CCD) was chosen as experimental design and optimization. The synthesized catalysts was used in the transesterification of oil with different FFA and the yield and the ester peak intensity (EPI) from the FTIR spectrum was used as response. Statistical analysis showed satisfactory description by a quadratic model, while the EPI was described by a 2FI model. The catalyst was then used on oil with FFA of 3.4; the resulting yield was 97.99% and an EPI of 0.789. Reaction parameter optimization was conducted with Neem oil having FFA of 3.4. Four factors was varied in the second phase of the experimental design; the reaction time, reaction temperature, catalyst weight, and oil-methanol mole ratio. Statistical analysis showed yield and EPI were described by separate quadratic models. 95.80% yield and EPI of 0.8601 were obtained after optimization and validation. On reuse of spent catalyst, the yield and EPI dropped to 84.3% and 0.782 respectively only after the sixth run, this was due to inefficient catalyst recovery as only 12% of the starting catalyst weight was recovered after the sixth run. The catalyst was then magnetized and the same reusability test was conducted, after the ninth run, the yield and EPI were 92.1% and 0.805 respectively, 46% of the starting catalyst was recovered. Characterization of the catalyst was done using SEM-EDS, XRD, BET and XRF.

### EP 16

**Preparation and application of KF/Eggshell Catalyst in Transesterification of Neem Oil**

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A strong solid base KF/Eggshell catalyst was prepared by wet impregnation method and applied for the circumvention of the occurrence of saponification during biodiesel production from high FFA vegetable oil. BET analysis revealed that, the catalyst has a specific surface area of 128 m\(^2\)/g, a pore size of 3.24nm and pore volume of 0.045 cm\(^3\)/g. Furthermore, the 79 nm sized crystallites of the catalyst having hexagonal shapes are shown in the SEM images to be systemically arranged; as such, present the high specific surface area of the catalyst to the reacting species. The parameters affecting the preparation of the catalyst such as calcination temperature and time of the eggshell, KF dosage, calcination time and temperature of the catalyst were investigated. The best synthesis conditions were found to be 900\(^0\)C eggshell calcination temperature for 4h, 30 wt. % KF dosage, and 600\(^0\)C KF/Eggshell calcination temperature for 4h. The catalyst was applied in a single stage transesterification of neem oil having FFA of 4.2% to produce biodiesel, 94.8% yield of biodiesel was obtained. Analyses of some important fuel properties indicated that, the biodiesel produced is comparable to the ASTM commercial standard for automobile applications.
### EP 17

**Morphology Optimization Of Solution Processed Perovskite Solar Cell**

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Organolead trihalide perovskite based solar cells have shown success as light absorbers in photovoltaic cells due to their efficiency increasing from 3.5% to over 20% within only five years. However, pinhole formation and incomplete coverage of solution processed perovskite film results in increased current leakage reducing efficiency. Hence the surface morphology of perovskite film is important for high performance of perovskite based solar cells. Here the morphology is carefully controlled by varying processing conditions, where drying at room temperature followed by double step thermal annealing were carried out at varying temperature and time. A mixed solvent of γ-butyrolactone and dimethylformamide (DMF) was used with chlorobenzene drop-casting during the spin coating process to reduce the surface defect. The optical absorbance of perovskite films was measured by UV-Vis Spectrometer, crystal structures of films were measured by use of X-Ray Diffractometer and spectra analysis was done using Fourier Transform Infrared Spectroscopy (FTIR). Surface morphology was measured using Scanning Electron Microscope which showed uniform and dense perovskite layer. The deposited perovskite films were free of pin-holes and highly uniform, the results gotten provides a clear understanding of the role of solution processing in achieving low-cost and high performance perovskite solar cell.

### EP 18

**Characterization of Nanocomposite Polymer Electrolyte for Solid State Electrochemical Application**

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Polymer electrolytes of PEO-MgO/NaSCN Nanocomposite were developed via a two-step reaction route involving synthesis of MgO Nanoparticles (NPs) by adopting microwave assisted co-precipitation method and subsequent mixing of MgO Nps and NaSCN (ionic charge supplier) with the host polymer matrix. Structural modifications resulting from the incorporation of MgO Nps and dispersion of NaSCN into the host polymer matrix (PEO) were studied using Fourier Transform Infrared Spectroscopy (FTIR). The transport properties of the nanocomposite polymer electrolytes (NCPEs) were carried out by measuring the conductivity and polarization for samples containing different wt% of MgO. Polarization and conductivity studies confirmed that the transference number and ionic conductivity increased with increasing MgO content (0-30%) of the NCPEs. However, a maximum conductivity of 5.3x10\(^{-4}\) S/cm and transference number of 0.88 were observed for sample containing 30wt% MgO. These properties show that the PEO-MgO/NaSCN electrolytes could serve as potential electrolyte for electrochemical applications.

### EP 19

**Optical and electrical characterization of Ni-doped CdS thin films prepared by Chemical bath deposition for solar Cell Application**

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In this study, the effect of doping on electrical and optical properties of CdS thin films prepared by Chemical Bath deposition technique has been investigated. The un-doped and Nickel-doped
Cadmium sulphide thin films were prepared by Chemical Bath deposition from aqueous solution of hydrated cadmium chloride (CdCl$_2$.21/$_2$H$_2$O) and thiourea (CH$_4$N$_2$S) respectively. Nickel (II) Chloride (NiCl$_2$.6H$_2$O) was used as a dopant and Triethanolamine (TEA) as a complexing agent while ammonia solution was used as the pH regulator. Thin films with varying Cadmium/Nickel percentage weight ratios (0%, 15%, 25% and 45%) were deposited on fluorine doped Tin oxide (FTO) glass substrates and microscope glass slide. The effect of Nickel concentration and annealing temperatures on the optical, electrical and structural properties of the deposited films was investigated.

The structural, compositional and optical properties of the deposited undoped and Ni-doped CdS thin films have been studied by X-ray diffractometer, energy dispersive X-ray Fluorescence spectrometer (EDXRF), UV–Vis and spectrophotometer respectively. Hall Effect measurements and work function measurements were also done using Hall Effect setup and a Kelvin probe. X-ray diffraction (XRD) analysis revealed that the un-doped and Ni-doped CdS thin films were polycrystalline with hexagonal structure. All films were found to be transparent while the transmittance in the visible region (400nm-700nm) varied between 40% and 60%, depending on the dopant concentration and the annealing temperature. The band gaps of Ni-doped CdS decreased with increased annealing temperature up to 250°C and increased with increasing annealing temperature beyond 250°C. The band gap increased with Nickel concentration and the band gaps (E$_g$) for the films prepared varies from 2.006 to 4.005 eV. The mean Work Function for as-grown CdS, 25%Ni-doped CdS and 45% Ni-doped CdS thin films were found to be -807.4 mV, -1141.9 mV and -953.5 mV respectively.

### EP 20

**Synthesis, Characterisation and Modelling of Cu$_2$ZnSnS$_4$ & Cu$_2$ZnSnSe$_4$ semiconducting nanocrystals for application in solar cells**

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Semiconducting nanocrystals also known as quantum dots (QDs) are among the third generation materials known as promising candidates for photovoltaic (PV) applications [1]. Third generation materials such as polymers, nanocrystals/quantum dots, organic material and perovskites are reported to be the immersing materials for solar cell fabrication [2-3]. Colloidal solution synthesis of QDs enables the simple and low cost production of thin film PV solar cells. In this study, quaternary copper zinc tin sulphur (Cu$_2$ZnSnS$_4$) abbreviated as CZTS and copper zinc tin selenide (Cu$_2$ZnSnSe$_4$) abbreviated as CZTSe nanocrystals have been synthesized using colloidal solution synthesis. The as-synthesized CZTS and CZTSe nanocrystals are composed of earth-abundant elements, which have been reported to exhibit a bandgap within the range 1.0–1.5 eV[4]. The nanocrystals were characterised using Ultraviolet-visible (UV-Vis) spectroscopy, Photoluminescence (PL), Powder X-ray Diffraction (PXRD), Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM). The characteristic PXRD peaks from CZTS (Figure 1a) illustrate the hkl planes to be (112), (200), (220), (312), (224) and (008) which are known to have kesterite crystal structure. Similarly, from CZTSe (Figure 1b) the planes illustrated are (112), (204), (312), (008) and (316).
An Intelligent Predictive Model for Energy Consumption in Institutional Buildings using Neural Network
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In the quest to achieving sustainable development in this 21st century, energy efficiency is paramount to achieving this goal. Statistics in recent research has shown that in many sectors which includes buildings, industries and transportation in any nation’s economy, energy consumption in buildings account for a higher percentage of about 40% unlike the other sectors in Nigeria and the world at large. Energy consumption forecasting is a critical and necessary input to planning and monitoring energy usage which further realizes to the worlds utmost fraction of CO2 alongside other greenhouse gas emissions. According to literature, very few research has been carried out in designing models for energy consumption in institutional buildings. In this research, the African University of Science and Technology (AUST) is considered as a case study, whereby the data being collected is the monthly energy consumption for a period of (2007 - 2017). A model is developed for the monthly prediction of energy consumption of the buildings within the university using ANN. Results obtained was compared with a regression model which showed that the ANN had a better predictive accuracy. This will further assist the university in monitoring the trends energy consumption, classify factors and components that impact energy consumption within the university community and hence building policies on its usage and consumption Moreover the possibility of using renewable energy (RE) in the university could also be integrated as future work.

Investigating the Corrosion Resistance of Spark Plasma Sintered Copper with Ruthenium Powder
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The world has a progressive increase in the need of electric storage and transfer facilities, which are highly dependent on copper (Cu). Copper is considered and preferred for use in such units because of its excellent electrical and thermal conductivity properties. It has industrial applications such as power cables, generators, heat exchangers, interconnects, and super capacitors. When copper is exposed in acidic environments containing sulfur, it tends to corrode compromising its function. The aim of this work was to increase the corrosion resistance of Cu by alloying it with ruthenium (Ru) using the spark plasma sintering (SPS) technique without compromising its electrical conductivity. Potentiodynamic polarization tests were performed to determine
improvement of the copper corrosion resistance. Pure Cu and Ru powders, 99.99% pure with particle size ranging from 10-45µm, were mixed using a turbular shaker. The spark plasma sintering process was used to produce the alloys using a FCT HP-D5 furnace. The alloys were ground and polished and used for corrosion testing. The response of the material to the potentiodynamic polarisation measurements were investigated in 2M H2SO4 solutions at 45 and 65°C. Polarisation curves were obtained and corrosion rates were calculated using the polarisation resistance technique. The corrosion resistance property of all copper alloys improved, when ruthenium was added, as compared to that of pure copper in sulfuric acid environments at 45°C and 65°C. The Ru added in the copper alloy resulted in finer grains in the grain structure of copper.

EP 23 Photovoltaics of Novel Highly Branched Organothiophenyl-Silane Polymers
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The increasing cost of fossil fuel as source of energy and its implication in environmental pollution and climate change created high demand for alternative and renewable sources of energy. This has led to great interest in research in the field of photovoltaic or solar cells. Solar cell is a device that converts sunlight into energy through the photovoltaic effect. The photovoltaic effect is the direct conversion of incident light into electricity by a semiconductor junction device. Due to the abundance of sunlight, the technology is sustainable, non-polluting and can be implemented at places where power demand is needed, for example in rural areas. Solar cell devices that have been commercialized are currently based on silicon technology, involving the use of monocrystalline, polycrystalline and amorphous silicon. Although they produce highly efficient solar cells, the cost of Si solar cells is too high. Second generation solar cell materials such as cadmium telluride and third generation materials such as perovskites and organic polymers have been receiving much attention recently. However, they lack the efficiency of Si solar cells. This research proposes the development of high energy conservation photovoltaic cells from novel low-cost organosilicon polymers. The aim is to develop novel highly branched Organosilane polymers such as Polydi(thien-2-yl)dimethylsilane, as electron donors (zinc oxide nanorod as acceptors) are able to bring the efficiency of the resultant photovoltaic cell close to that of Si solar cell as well as the band gap. The zinc oxide nanorods are prepared by wet chemistry methodology involving the use of zinc acetate and sodium hydroxide and absolute ethanol. The testing of the materials for photovoltaic effects involve the assembly of the donor Organosilane polymer and acceptor ZnO nanorods into a bulk heterojunction photovoltaic device.

EP 24 Nanostructured hybrid olivine materials for advanced lithium ion battery cathodes
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Lithium ion batteries have been dominating in consumer electronics and are slowly tapping into electric and hybrid electric vehicle applications. However, the requirements for high energy and power densities, limits the full exploration of these batteries in heavy duty applications [1]. The cathode material, a key component in lithium ion batteries is made up of a single material which makes it challenging to meet all the requirements of a superior cathode material [2]. Recent works have shown that a combination of two cathode materials that complement each other’s properties will perform better that the individual cathode material. This work is based on the synthesis and the characterization of graphene coated lithium iron phosphate-lithium manganese silicate hybrid cathode material to be considered for use in lithium ion batteries. LiFePO4 is a desirable cathode material with several advantages such as long cycle life, relative high specific capacity (170 mAh/g), and excellent electrochemical and thermal stabilities [3]. Complementary, Li2MnSiO4 will offer its high specific capacity (330 mAh/g), which is twice that of the former. The added advantage of blending these materials is that they are off low cost, environmentally friendly and less toxic.
However, the insulating nature of these materials limits them from reaching their theoretical capacities. The incorporation of graphene nanosheets, a material with excellent chemical stability and superior electric and thermal stabilities associated with its high charge carrier is expected to suppress the challenge encountered by these materials [4]. The physical and electrochemical properties of the hybrid material will be investigated using: (i) X-ray Diffraction, (ii) Solid State Nuclear Magnetic Resonance Spectroscopy (iii) High Resolution Scanning, and (iv) Transmission Electron Microscopies, (v) Energy Dispersive Microscopy, (vi) Fourier Transform Infra-red Spectroscopy, (vii) Small Angle X-ray Scattering, (viii) Cyclic Voltammetry and (ix) Electrical Impedance Spectroscopy.

<table>
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<th>EP 25</th>
<th>Effect of the thickness of copper doped nickel oxide hole transport layer on the performance of planar CH$_3$NH$_3$PbI$_3$ perovskite solar cells</th>
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<tr>
<td>D.M. Sanni$^{1,3,4}$, A. Yerramilli$^3$, Y. Chen$^4$, J. Asare$^4$, E. Ntsoenzok$^{2,5}$, T. Alford$^{2,3}$</td>
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<tr>
<td>$^1$African University of Science and Technology (Department of Theoretical and Applied Physics, Abuja, Nigeria)</td>
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<tr>
<td>$^2$African University of Science and Technology, (Department of Material Science and Engineering, Abuja, Nigeria)</td>
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<td>$^3$Arizona State University (School for Engineering of Matter, Transportation and Energy, AZ, 85282, United States)</td>
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In a planar perovskite solar cell, poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) is commonly used as the hole transport layer (HTL). However, its acidity and tendency to absorb water causing poor long-term stability hence, the need for alternative hole transport layer. In this study, solution-processed copper-doped nickel oxide was synthesized for use as hole transport layer (HTL) in the fabrication of planar perovskite solar cell devices. The copper-doped nickel oxide thin films were deposited using spin coating technique and they were post-annealed at 500 °C. The spin coating rate was varied to investigate how it will affect the photovoltaic performance and the optical properties of the planar perovskite solar cell. It was observed that as the thickness increases at a lower spin rate the optical transmittance reduces and the conductivity increases. The planar perovskite-based solar cells with solution-processed copper-doped nickel oxide as the hole transporting layer have better short-circuit current density ($J_{sc}$), open circuit voltage ($V_{oc}$), and power conversion efficiency (PCE) at a spin rate of 3000 r.m.p. The thickness of copper doped nickel oxide film, however, has no effect on the photo-stability of the fabricated solar cell devices.

<table>
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<th>EP 26</th>
<th>Voltage Holding a Reliable Technique for Evaluating the Cycling Performance of Supercapacitors in Aqueous Electrolyte</th>
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<tr>
<td>A Bello$^{1,2,*}$, F. Barzegar$^2$, M. J. Madito$^2$, D. Y. Momodu$^2$, A. A. Khaleed$^2$, T. M. Masikhwa$^2$, J. K. Dangbegnon$^2$ and N. Manyala$^2$</td>
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<td>$^1$Department of Materials Science and Engineering, African University of Science and Technology (AUST), Abuja, Federal Capital Territory, Nigeria</td>
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<td>Email: <a href="mailto:abello@aust.edu.ng">abello@aust.edu.ng</a></td>
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Supercapacitors (SCs) have attracted significant interest for the development of next generation of energy storage systems. They are characterized by their high power density and low energy density when compared with batteries and are suitable for transient energy saving application such as energy capture during braking in vehicles and for opening of doors in the A380 Jumbo jet. However, the performance of SCs devices is exclusively dependent on the physicochemical properties of the
Electrode materials with diverse dimensionalities such as 1D, 2D and 3D nanostructures have been explored to improve supercapacitive properties by taking advantages of the unique ability of the different nanostructure for ion propagation and charge storage. The stability of supercapacitors is a very important feature for true and practical application of ECs devices. The conventional method for evaluating the stability is through the continuous cycling of the device at a constant current over thousands of cycles which in many cases does not show degradation to the devices. As an alternative or complement to this approach floating technique based on voltage holding been proposed as a reliable technique to test the stability of electrode materials. Thus, the performance (specific capacitance) of symmetric capacitors based on mesoporous polymer derived carbons and the stability of the symmetric capacitors based on voltage holding (floating conditions) operating in aqueous electrolyte is reported. Variation in the specific capacitance values with the floating conditions shows a good cycling life performance in alkaline electrolyte for ~500 h (three weeks).

**EP 27**

**Doped Few Layer Graphene (FLG) as Transparent Conducting Electrode for OLEDs**

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Graphene based transparent conducting electrodes (TCE) are attracting research interests for applications in organic light emitting diodes (OLEDs) and organic photovoltaics (OPVs). This is owed to the superb properties of graphene such as outstanding electrical and optical properties. The application of graphene as TCE material is limited to its high sheet resistance and the inappropriate work function mismatch which limits the hole injection from the pristine graphene anode to an adjacent layer and considerably affects the performance of OLEDs. Charge transfer doping of graphene has emerged as one of the ways to lower the sheet resistance of graphene without sacrificing the optical transmittance of the graphene. In this work, we developed TCEs based on surface doped few layer graphene (FLG). The charge transfer doping were achieved by spin coating two transition metal oxides MoO₃, V₂O₅ dissolved in H₂O₂ and AuCl₃ dissolved in nitromethane on the CVD grown graphene on Si/SiO₂ substrate. The sheet resistance and optical transmittance of samples doped with MoO₃, V₂O₅ and AuCl₃ were compared. Thermal stability and environmental stability of these dopant chemicals were also studied. We also fabricated an OLED device based on the sample with most outstanding combination of properties. This led to a device with efficiency comparable and even higher than the previously reported values.

**EP 28**

**Application of the Quantum ESPRESSO Code To Study The Structural and Electronic Properties of Silicon Carbide (SiC), A Solar Cell Material For Environments With High Temperature.**

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Energy problems are being faced in different forms in various parts of the world. In most parts of Africa, the major problem is that of shortage of energy supply while in industrialized countries, there exists the problem of pollution. Over the years, there have been so much efforts by researchers all over the world to harness the sun’s energy as an alternative, as it solves the problem of accessibility and is a clean source of energy. Silicon Carbide (SiC), a IV-IV binary compound semiconductor is known to be very hard, mechanically resistant and chemically stable. It crystallizes in several forms, which gives it more versatility. In the Zinc-Blende phase, SiC has an experimental wide band gap (about 2.39 eV), which makes it more efficient than silicon at high temperatures. It’s thermal conductivity is also higher compared to that of GaAs These properties make SiC a material that can readily be used in solar cells, especially in high temperature regions. Besides this,
SiC based inverters are known to operate at very high efficiency. This study seeks to predict the preferred crystal structure and structural properties of SiC from first principles. Total energy ab initio calculations have been performed under the framework of the density functional theory (DFT). A standard scheme has been followed using UltraSoft pseudopotentials and the Perdew–Burke–Ernzerh (PBE) exchange–correlation functional downloaded from the Quantum Espresso Library. The band structure, density of state and enthalpy-pressure calculations lead to the conclusion that SiC undergoes transition from indirect band gap semiconducting (WZ or ZB phase) to metallic nature (RS phase) at the structural transition pressure with a volume reduction of about 19.7%. Zinc Blende phase being slightly more stable than wurtzite is the most stable of the three phases of Silicon Carbide studied.

EP 29  Electrochemical and Charge Storage Properties Of Polyaniline/ Polyimide Thin Films
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Polymer solar cells offer numerous advantages over silicon-based. Major obstacle to using polymers for solar cells is their processability and the difficulty in the quantitative assessment of the polymer performance within the organic solar cell. Polyaniline is by far the most important conducting polymer from the point of view of large scale technological use. The resultant synergy from blending an intrinsically conducting polymer like polyaniline (PANI) an organic polymer that possesses the electrical, electronic, magnetic and optical properties of a metal while retaining the mechanical properties, solubility, processibility commonly associated with a conventional polymer, with an aromatic polyimide possessing outstanding thermal, mechanical, electrical, and solvent resistance properties overcomes the poor mechanical properties and instability of the conducting polymers. In this study, we have proceeded to blend the single polymers i.e. PANi and Polyamic Acid (PAA) in three different ways this includes layer by layer deposition, in situ homogeneous blending and drop coating methods. In this we have identified the best approach for blending. As well as determining the ideal approach to utilise in the impedance analysis and characterisation of materials suitable for semi-conductor organic photovoltaic cell applications. This study has shown that specific capacitances of polymer blends of PANi and PAA estimated using various techniques as well as the effectiveness of impedance studies in deducing the system parameters from the fitting of the equivalent circuit data. Electrochemical evaluation by DC and AC voltammetry allowed us to quantify the charge transfer and charge storage properties of these materials and explore their potential application in the design as cheap, robust environmentally stable alternative energy sources as can be used in solar cells/ capacitors.

EP 30  Photovoltaics of Copper Telluride Dendritic Core-Shell Nanoparticles
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The demand of energy in present society is continually increasing. The need for energy resources which are environmentally friendly as alternative for fossil fuels energy resources is growing. Photovoltaic (PV) energy is an important technology and is progressing to attract a great attention from PV community due to their advantages such as no fuel cost, environmentally friendly, low fabrication cost, easy to fabricate, etc. Currently, there are research activities focussing on finding ways to improve their efficiencies and long term stability. In this study, dendritic core-shell nanoparticles (Core-Shell NPs) were synthesized using copper telluride nanoparticles (CuTe NPs) as a core material and 5-(2-thienyl) salicyldimine dendrimer (First generation) as a shell material
which were used as acceptor material. CuTe NPs were synthesized via chemical reduction and 5-(2-thienyl) salicylaldimine dendrimer were synthesized Schiff base condensation between Polypropylenimine tetramine dendrimer (DAB-Am-4) and 5-thienylsalicylaldehyde. Core-Shell NPs were characterized by UV-Vis spectroscopy were they broad and red shifted bands as compared to the bands from the UV-Vis spectrum of 5-(2-thienyl) salicylaldimine dendrimer, transmission electron microscopy (TEM) and small- and wide-angle X-ray scattering experiments confirmed that the synthesized particles are Core-Shell NPs. The Core-Shell NPs were blended with poly[N-9′-heptadecanyl-2,7-carbazole-alt-5,5-(4′,7′-di-2-thienyl-2′,1′,3′-benzothiadiazole)] (PCDTBT) as a donor material and their optical properties were studied with UV-Vis and photoluminescence spectroscopies. The UV-Vis spectrum of PCDTBT blended with Core-Shell NPs showed a new band at ~830 nm which indicates that the Core-Shell NPs have band gap characteristic that make them suitable for photovoltaics application.

**EP 31**

**Solar Photocatalytic Hydrogen Production via Glycerol Reforming Over Transition Metals Supported TiO2 Hollow Spheres: Preparation, Characterization, and Photoactivity.**

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Nanostructured TiO\(_2\) hollow spheres (THS) were prepared via a simple hydrothermal method with titanium butoxide, ethanol, urea, and ammonium sulphate. The effects of Ti/ethanol, and reflux temperature on the morphological properties of the nanostructured TiO\(_2\) hollow spheres were investigated. An impregnation method was subsequently employed to load transition metals such as Cu, Co, Cr, Ag, and Ni on the optimized TiO\(_2\) hollow spheres, followed by calcination in H\(_2\)/N\(_2\) at 450 °C for 4 h. The morphological properties of the prepared samples were characterized by Brunauer-Emmett-Teller (BET), X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and UV/vis. The SEM and TEM pictures showed that the Ti/ethanol ratio of 1:10 resulted in the formation of uniform hollow spheres. The XRD spectre revealed that phase transformation took place as the reflux temperature was increased, with pure anatase TiO\(_2\) hollow spheres being formed at 200 °C. The BET surface areas of the calcined photocatalysts were in the range of 80.6 – 116 m\(^2\)/g. The UV/vis spectra of the photocatalysts showed that loading of transition metals reduced the band gap of the TiO\(_2\) hollow spheres. The activities of the prepared catalysts were tested for hydrogen production via photocatalytic reforming of glycerol under solar irradiation. The improved hydrogen evolution from photocatalytic reforming of glycerol was attributed to: the high surface area which enhanced the adsorption of glycerol onto the surface of photocatalysts; high crystallinity and the reduced band gap which improved the solar light harvesting; the hollow chamber within the TiO\(_2\) spheres which produced multiple reflection of the light harvested, thus producing efficient electron/hole pair formation, and the detailed composition of the solids retarded the electron/hole recombination by trapping the electrons generated during the photo excitation of the photocatalysts, and thereby promoted their activity.

**EP 32**

**Investigation of lithium vanadium phosphates as a cathode material for lithium-ion batteries**

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The aim of this investigation is to synthesis and characterize a lithium vanadium phosphate with good capacity and a high voltage. A wide range of studies have been carried out to investigate the structure and properties of lithium compounds that are suitable for use in lithium-ion batteries.
Lithium is useful as it has one of the smallest ionic radii and possibly the highest cell potential. Phosphates have exhibited noteworthy operating potentials and high thermodynamic and kinetic stability. Vanadium has the advantage of tuning its oxidation state from $V^{2+}$ to $V^{5+}$. Combination of these three components promises a cathode material that will possibly possess high lithium capacity, good ion mobility, a good capacity and a high operating voltage of approximately 4.0 V. Synthesis methods include hydrothermal synthesis or a combination of grinding and annealing. Techniques useful for characterization of the cathode material include powder x-ray diffraction (PXRD), thermo-gravimetric analysis (TGA), transmission electron microscopy (TEM) and electrochemical testing that includes galvanostatic charge-discharge, cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS).

**EP 33**

**Photophysics of Novel Electroresponsive 3-Dimensional Poly(Propylene Thiophene)-Co-Poly(3,4-Ethyleneedioxythiophene) Dendritic Copolymer**

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This project seeks to develop a new class of photovoltaic devices, based on the current proposed fourth generation solar PV cells however utilizing cheap, and conductive star co-polymer made on the basis of innovative dendrimer chemistry; hence reducing the cost of solar cells and improving the properties of the dendritic star copolymers compared to those made in the basis of typical two-dimensional linear polymers approach. In this way we expect to make a very important improvement on the efficiency of the dominant solar photovoltaic technology. This was achieved by synthesizing separately the parent materials (functionalized 3-dimensional poly(propylene thiophene) dendrimer and the two-dimensional poly(3,4-ethylenedioxythiophene)) and later copolymerised oxidatively using iron chloride as the oxidising agent to form the star co-polymer, poly(propylene thiophene)-co-poly(3,4-ethylenedioxythiophene). Structural characterization of the materials XRD, UV-Vis/photoluminescence, TGA and FTIR/H$^1$ NMR to investigate material crystallinity, optical properties, thermal stability and chemical structure, respectively. The electrochemistry of the materials was studied by cyclic voltammetry (CV) and square wave voltammetry (SWV). $^1$H NMR and FTIR confirmed that poly(3,4-ethylenedioxythiophene) was incorporated into the dendrimer moiety through $\alpha - \alpha$ coupling on the thiophene ring with the disappearance of $\alpha - \alpha$ hydrogens [1]. XRD results revealed the amorphousness of the materials with an observed characteristic broad peak at 26° [2]. TGA indicated that the copolymer is more thermally stable than poly(3,4-ethylenedioxythiophene) but undergoes structural degradation at elevated temperatures. The materials were found to be electro-responsive with low oxidation potential ($< 0.2 V$) and HOMO and LUMO properties of a semiconductor.

**EP 34**

**Biodiesel production by Transesterification of waste cooking oil using modified Attapulgite**

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Biodiesel is a renewable and an alternative fuel for diesel engines due to its non-toxicity, biodegradability and its ability to reduce greenhouse gases. The aim of the study is to produce biodiesel from waste cooking oil using heterogeneous catalyst. The heterogeneous catalyst was prepared by ion-exchange method. The biodiesel was prepared using transesterification reaction, which is a reaction whereby methanol is mixed with oil in a 3 is to 1 ratio in the presence of a catalyst.
The parameters that influences the transesterification reaction were investigated. Such parameters include reaction temperature, reaction time, methanol/oil ratio, catalyst amount and stirring rate. The results showed that the biodiesel yield increased with the increase in the reaction parameters. 94% yield of biodiesel was obtained when 1:9 ratio and 5g catalyst were used for at 70°C for 5 hours at a stirring rate of 500rpm.

**EP 35**

**Perovskite Solar Cells with PEDOT/NiO\textsubscript{x} Composite Hole Injection Layer**  
J. Asare\textsuperscript{1,2,3}, A. S. Yerramilli\textsuperscript{2}, Y. Chen\textsuperscript{2}, D. M. Sanni\textsuperscript{2,3}, T. L. Alford\textsuperscript{2,3}

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A new hole transportation layer (HTL) combined with PEDOT:PSS and Copper doped Nickel Oxide (Cu:NiO\textsubscript{x}) in Perovskite-based solar cells (SCs) is fabricated. Cu:NiO\textsubscript{x} thin films are prepared on Fluorine-doped Tin Oxide (FTO) glass substrates using a solution containing Nickel acetate tetrahydrate, 2-Methoxyethanol and Monoethanolamine (MEA) and Copper acetate monohydrate. After that PEDOT:PSS are prepared on Cu:NiO\textsubscript{x} forming the composite hole transportation layer. The organic-inorganic CH\textsubscript{3}NH\textsubscript{3}PbI\textsubscript{3} active layer derived from Pb-acetate based solution, [6,6]-phenyl C\textsubscript{61}-butyric acid methyl ester, and Al electrode are subsequently deposited, forming the inverted planar SC. PCE values higher than 10% can be realized using this low-temperature anneal process. Effects of anneal temperature and solution concentration on the properties of the SC are elucidated. Stability of the SC based on PEDOT/NiO\textsubscript{x} composite HTL is explored compared to the stability of SC using single PEDOT HTL.

**EP 36**

**Effect of Low Temperature Annealing on the Photovoltaic Properties of Perovskite Solar Cells Using Dehydrated Lead Acetate Precursor**  
D.M. Sanni\textsuperscript{1-4}, Y. S. Chen\textsuperscript{3}, A. S. Yerramilli\textsuperscript{3}, J. Asare\textsuperscript{4}, E. Ntsoenzok\textsuperscript{2}, T. L. Alford\textsuperscript{2,3}

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In this study, we reported a low-temperature annealing process to fabricate perovskite solar cells (PSC) using dehydrated lead acetate (Pb(OAc)\textsubscript{2}) and methylammonium iodide (MAI) as the source materials. We vary the concentrations of the methylammonium iodide and dehydrated lead acetate as well as varying the post-deposition annealing temperature of the perovskite active layer. The inverted planar (n-i-p) perovskite solar cell architecture was adopted, using PEDOT:PSS as the
hole transport layer and phenyl –C61-butyric acid methyl ester (PCBM) as the electron transport layer. We investigated the effect of low annealing temperature on the optical and structural properties of the film and the photovoltaic performance of the fabricated solar cell devices. We recorded a power conversion efficiency higher 12% at an annealing temperature below 100 °C.

**EP 37**

**Platinum-tin nanoparticles supported on carbon nanodots as efficient anode electrocatalysts for direct ethanol fuel cells**

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Energy is basic need in our everyday lives. Non-renewable energy sources such as coal and gasoline will not satisfy the growing energy demands. Furthermore, the extraction and processing of some these non-renewable pose some environmental concerns such as air pollution and global warming. Therefore, there is a need to develop sustainable energy sources such as fuel cells. South Africa is the world second largest producer of platinum that can be used as electrocatalysts for fuel cells. Platinum is the most active electrocatalyst for acidic direct alcohol fuel cells (DAFC). However, it is easily poisoned by the intermediates formed during the alcohol oxidation reactions (AOR). The activity of platinum-based electrocatalysts can be improved by: (i) alloying platinum with a cheaper metal such Sn, Ru and Co and (ii) using a support material with high surface area which helps to enhance the catalyst dispersion. In this work, carbon nanodots (CNDs) with 312.5 m²g⁻¹ BET surface area, 9.64% oxygen content and particle sizes between 1-8 nm were synthesized using a cheap and green method. The Pt-Sn nanoparticles were deposited on to the CNDs to produce an electro active catalyst with low poisoning rates.

**EP 38**

**Optical Characterization of Transparent Porous Polymer Based TiO₂ Thin Films for Nanocrystalline Solar Cell Applications**

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Energy is vital for development of any country. With new gadgets consuming power appearing the market at a high rate, there is need to think beyond the current energy sources. Material properties can be determined by many factors, composition being a major factor. In this study, we explore the optical properties of polymer based TiO₂ films for photovoltaic applications. TiO₂ films incorporating Polyvinylidene Fluoride-Co-Hexa fluoropropylene (PVDF-HFP) as the structure directing polymer and using Titanium Isopropoxide as the precursor were deposited by both dipping and spin coating techniques. The films were optimized with respect to solution concentration, and spin coater speeds as well as dip coating with drawal speed. X-Ray diffraction (XRD) structural, as well as transmittance studies were carried out. XRD spectra showed crystalline anatase films with crystal sizes of about 18-24 nm after annealing at about 450 °C for 30 minutes. The as deposited films were amorphous. The films showed low refractive index and significant porosity making them suitable for nanocrystalline solar cell applications.

**EP 39**

**Activated Carbon Derived from Plant Biomass Materials for Mixed Assembly Supercapacitors**

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Activated carbon (AC) was obtained from three different plant biomass wastes sources (coconut shell, pine cones and rice husk) via hydrothermal treatment followed by carbonization at 800 °C. The morphological and structural characteristics of the transformed carbon material revealed a porous network suitable for energy storage application. The asymmetric cells fabricated exhibited EDLC behavior in all material sample combinations using all three transformed activated carbons. The mixed assembly device worked comfortably in a voltage window of 1.5 V in a neutral electrolyte. A specific capacitance (CS) of ~110 F g⁻¹ was obtained with a corresponding energy density of 8.5 W h kg⁻¹ and power density of 380 W kg⁻¹ at a current density of 0.5 A g⁻¹. An excellent stability was exhibited with a coulombic efficiency of a 99.7% and capacitance retention of 80% after 10000 continuous cycling at 5.0 A g⁻¹. Furthermore, subjecting the device to a floating test for ~48 h (2 days) at the optimum voltage (1.5 V) revealed a drop in the initial capacitance value but still without any recorded device failure. Remarkably, the asymmetric design showed a potential for adopting EDLC materials of different carbon sources in order to capture the entire properties for efficient and stable energy storage devices.

**EP 40 Preparation And Characterization Of Nanostructured Nickel Doped Zinc Oxide (Ni:Zno) Thin Film For Solar Cell Application**

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Nanostructured Nickel doped Zinc Oxide thin films have been deposited on soda lime glass and indium tin oxide (ITO) coated glass slide coated substrates by chemical spray pyrolysis technique (CSP). The influence of the Ni doping on the surface morphological and optical and electrical properties of the thin films were investigated using SEM with EDX, uv-vis spectrophotometer, keithley source meter 2400 coupled with four point probe and the I-V measurement in dark for the purpose of fabricating cheap, high efficient and environmental friendly Optoelectronic devices such as solar cell, LED etc.

Morphological studies revealed that the films were continuous and the particles were uniformly distributed across the substrate’s surface with crystal size decreases with the present of Ni dopant. EDX indicates that the presence of Zn and O of ZnO film and Ni, Zn and O in the Ni:ZnO film with little or no impurities. Optical analysis of Ni:ZnO thin films gave high optical absorption in the uv-visible region. The band gap obtained ranged from 3.05 eV to 3.15 eV with a good rectifying properties.

**EP 41 High temperature corrosion of Ru alloyed 304L stainless steels**

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Recently, it has been reported that high repair costs in thermal power plants are due to corrosion related problems. The tubing found in boilers and heat exchangers are often replaced before their expected life span because the corrosion properties are compromised at high temperatures. The passive film on the surface of stainless steels deteriorates and this leads to enhanced pitting and other forms of localised corrosion. Type 304L stainless steel becomes susceptible to corrosion when exposed to environments with high oxygen concentration in the presence of chlorides at elevated temperature. It is for this reason that this paper was focused on improving the corrosion resistance of 304L stainless steel by bulk alloying with Ru. Vacuum arc remelting technique was used to
prepare the samples. A 304L stainless steel coupon weighing 70 g was melted with Ru at varying contents 0, 0.5, 1, 2, and 5 wt%. The electrochemical test was then conducted in 50 ppm sodium chloride containing dissolved oxygen at 25 and 200°C. The potentiodynamic polarisation was performed at scanning rate of 0.1 mV/s. The laboratory results showed that additions of Ru improved the corrosion resistance significantly. The corrosion rates were lower for samples with lower Ru contents (i.e., below 1 wt%) when compared to as-received 304L stainless steel. However, higher levels of Ru (2 and 5 wt%) added did not improve the corrosion resistance and the current density was higher when compared to as-received 304L stainless steel.

**EP 42**

**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.¹ 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.³ 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 borophosphates 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 characterized 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.

**EP 43**

**Investigation of Ion Beam Modified CZTS (Cu₂ZnSnS₄) Thin Films for Photovoltaic Applications**
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This study focuses on investigating the properties of Cu₂ZnSnS₄ (CZTS) thin film materials modified by ion irradiation. CZTS is a quaternary semiconductor that has emerged as a promising candidate for low-cost thin film solar cells because of its suitable direct band gap of between 1.4 and 1.5 eV and large absorption coefficient of over 10⁴ cm⁻¹ [1]. Moreover, the abundance and low toxicity of the elements in the compound CZTS make it a future photovoltaic material of choice compared to the currently used compounds, such as copper indium selenide (CIS), copper indium gallium selenide (CIGS) and cadmium telluride (CdTe) which are rare and toxic [2]. However, the suitability of CZTS materials under different radiation environments has not yet been tested. CZTS thin films of 1 µm thickness were irradiated with H⁺ ions of energy 6.0 MeV at fluences, 5 × 10¹⁵, 1 × 10¹⁶, and 5 × 10¹⁷ ions/cm² to modify their properties. Structural, electrical and optical properties of pristine and ion beam modified CZTS films, characterized by X-ray Diffraction (XRD), Photoluminescence (PL) spectroscopy and Cathodoluminescence (CL) spectroscopy will be presented.
Investigation of post deposition annealing temperature effect on the performance of dehydrated lead acetate precursor in an inverted planar CH$_3$NH$_3$PbI$_3$ perovskite solar cells

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The highest power conversion efficiency (PCE) of perovskite solar cells (PSCs) employed the regular (n-i-p) architecture which has PCE of over 22%, but this is achieved by a thick layer of mesoporous TiO$_2$ which require high-temperature post-deposition annealing. In this work, we employed the inverted planar (n-i-p) perovskite solar cell architecture using a low-temperature annealing process. The hole transport layer is poly(3,4-ethylenedioxythiophene): poly(styrene sulfonate) (PEDOT: PSS); methylammonium iodide (MAI) and dehydrated lead acetate were the precursor materials for the perovskite layer and phenyl-C$_6$1-butyric acid methyl ester (PCBM) as the electron transport layer. In this work, we vary the concentrations of the methylammonium iodide and dehydrated lead acetate and we also investigated the effect of post-deposition annealing temperature of the perovskite active layer on the photovoltaic performance. We obtained power conversion efficiency (PCE) over 12% at annealing temperatures lower than 100°C.
### NP 01
**Improving the solid state fluorescent of perylene diimide using bulky nanoparticle at imide and a halogen at the core**  
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Jimma University, (School of materials science and engineering, Jimma, Ethiopia)  
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Perylene diimide (PDI) and its derivatives exhibit very good photophysical properties making them organic material of great interest for optoelectronic applications. However, these properties are only good in dilute/solution state and tend to weaken on aggregation/solidification. There is need to research in PDI materials with high photophysical properties specifically fluorescence emission solid state. We have synthesized a highly soluble and fluorescent perylene diimide dye substituted at the imide positions with POSS nanoparticle and bromine at the core (thereafter named 1) studied its properties both in solution and solid state in comparison to other three derivatives (2- ordinary PDI with linear alkyl chain, 3- similar to structure 2 but with bromine substitution at the core, 4- similar to structure 1 but without bromine core substitution). Concentration-dependent UV/vis absorption studies has been used to study aggregation behavior, crystals of 1, 2, 3, and 4 have been formed using slow bisolvent method and tested for fluorescent quantum yield ($\Phi_f$) using fluorescence emission spectroscopy. Molecular design 1 could only show signs of onset aggregation at high concentration of the order $10^{-4}$M unlike the other molecular structures 2, 3 and 4 which aggregated at lower concentration of $10^{-6}$M and below. Like any other PDI derivative, the solid state $\Phi_f$ of sample 2, 3 was very low 12% and 17%. POSS substitution alone (structure 4) increased to 48%. Introducing bromine at the core of PDI with POSS (structure 1) greatly improved the $\Phi_f$ to 83.5%. Both imide substitution with POSS and core substitution with bromine actively contributed to significant improvement of $\Phi_f$.

### NP 02
**Magnetic V-Hybrids (α-γ)CoV_2O_6 nanorods based photocatalyst systems**  
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$(\alpha – \gamma )\text{CoV}_2\text{O}_6$ Nanorods have been well synthesized using hydrothermal method. They exhibit monoclinic and triclinic phases with crystalline structures which are confirmed using XRD technique. The susceptibilities, magnetization and heat capacity are investigated showing that the material has antiferromagnetic properties. The successful degradation of Fuchsin dye at different time is also reported with a high percentage of degradation.

### NP 03
**Preparation and properties evaluation of biobased polyurethane - graphene nanocomposites**  
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Graphene consists of a 2-D layer of sp$^2$ hybridized carbon atoms with unique physical, chemical and mechanical properties that would allow the preparation of composite materials with outstanding characteristics. In this report, graphene was prepared from graphite powder by exfoliation in an aqueous ethanol, dispersed in polyhydroxylated rubber seed oil and the resultant hybrid was reacted with disocyanates (hexamethylene disocyanate and 4,4$^1$-methylene-bis(phenylisocyanate) in the presence of dibutyltin laurate catalyst. The morphology of the nanocomposite materials determined by x-ray diffraction (XRD) revealed that; the nanocomposites were largely amorphous with degree of crystallinity about the same order as in the unfilled polyurethanes; and that the graphene particles were well dispersed in the composite materials. Surface topology of the nanocomposite was determined by atomic force microscopy (AFM) and it revealed surface roughness, with average depth of the asperities higher for the nanocomposites (10.1 – 21.8 nm) than for the unfilled polyurethanes (7.1 – 19.3 nm). FTIR absorption bands were observed at about 1800cm$^{-1}$ (1785 – 1800cm$^{-1}$) in the spectra of the nanocomposite materials, were absent in the unfilled polyurethanes, suggesting graphene - polyurethane interaction. Physico - mechanical properties: modulus, elongation at break, ultimate tensile strength, yield stress, hardness and degree of swelling (in toluene) were found to be markedly enhanced in comparison with the unfilled polyurethane samples. Similar marked improvements in the thermal stability of the nanocomposite materials in comparison with the unfilled polyurethane samples were observed.

**NP 04** Laser Induced Breakdown Spectroscopy (LIBS) generated plasma in air containing carbon, nickel An yttrium target: temporal and spatial studies  
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$^4$Materials Research Department, iThemba LABS-National Research Foundation, 1 Old Faure Road, Somerset West 7129, PO Box 722, Somerset West, Western Cape Province, South Africa  
Email: mani@tlabs.ac.za  

Laser-induced breakdown spectroscopy (LIBS) is a type of atomic emission spectroscopy which uses a highly energetic laser pulse as the excitation source. The laser is focused to form a plasma, which atomizes and excites samples. The formation of the plasma only begins when the focused laser achieves a certain threshold for optical breakdown, which generally depends on the environment and the target material. In principle, LIBS can analyse any matter regardless of its physical state, be it solid, liquid or gas. In this work, plasma generated fundamental radiation from a Nd: YAG laser focused onto a graphite target is studied by spectroscopically in atmospheric pressure. The emitted particles ions or atoms or molecular species are short-lived, localized plasma, characterized by laser induce plasma spectroscopy. In this, study the interaction for graphite targets, laser-induced plasma (LIP) characteristics were examined in detail with the use of a space and time resolved method. Stark broadened profiles of singly ionized species have been utilized for electron density measurements ($N_e$). Relative line intensities of successive ionization states of carbon were used for electron temperature ($T_e$) calculations from the Boltzmann plot. The emission carbon and nickel elemental species electron temperatures in the range of 10 -19 ×10$^3$ K and ionic temperatures of 1 - 3 ×10$^3$ K with electron number densities of the order of 10$^{16}$ cm$^{-3}$ were observed. Electron temperature and density were studied as function of distance and time elapsed after the incidence of laser pulse. The fundamental approaches developed to analyse laser-target (i.e. solid graphite with Ni+Y metal catalyst) interaction, plasma generation as well as and its expansion will be reviewed, and compared with the standard NIST data.

**NP 05** Rapid Free-Electron Initiated Selective Polymerization At Room Temperature  
Boyce Chang, Stephanie Oyola-Reynoso, Jiahao Chen, Mingchang Lu, Martin Thuo*
The demand for polymers with intricate architecture expands with the advent of new applications using these materials, thus, leading to the discovery of novel methods for their production. Although the field of polymer synthesis has been extremely active, very few methods have been applied in industries due to their complexity and stringent requirements. We demonstrate the application of solvated electrons for rapid and selective polymerization of commercially available monomers at room temperature. The mechanism involving this method has been largely misunderstood due to an overgeneralized assumption made in the past. We first verify the inconsistent reports in literature regarding monomer selectivity and then provide evidence for a bi-mechanistic polymerization via radical anions. We show that the skewness of the molecular weight distribution can be employed to track initiation rate, which is crucial for the survival of the radical anions. This method is then further employed as a straightforward approach for producing block copolymers.

**NP 06**

**Photoionization cross section of hydrodenic impurities in cylindrical quantum dots within an infinite potential barrier**

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We have carried out a theoretical study of the dependence of photoionization cross-section on the incident photon energy for a hydrogenic donor impurity in a GaAs quantum dot of cylindrical cross-section. In this study we have employed a trial wave function for donor impurity in the effective mass approximation and assumed that the barrier potential is infinite. We find that the photoionization cross-section increases rapidly with incident photon energy up to a peak and then decreases slowly, almost monotonically. For a constant quantum dot radius, the cross-section is much larger for longer axial (z) dimension of quantum dot than for the shorter one. We also find that the photoionization cross-section varies with the donor impurity position along the dot axis, with the maxima of the cross-sections occurring at different impurity dot positions. Furthermore, the maxima of the photoionization cross-sections are not equal. This knowledge of the dependence of photoionization cross-section of the quantum dot on photon energy should be of great value for in understanding the optoelectronic properties quantum dots when designing optical devices using quantum dots.

**NP 07**

**Investigations of the effect of Nickel and Tin addition on the microstructure and mechanical properties of Aluminium – 4% Zinc alloy**

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This work investigated the effect of microalloying on the microstructure and mechanical properties of Al-4%Zn alloy. The mechanical properties studied were yield and ultimate tensile strength, % elongation, compressive strength and hardness. The tests were conducted using the ASTM E8, E10 and E20 standards. Microstructural analysis was done using metallurgical microscope model Olympus PMA–3 and the micrographs were obtained with an attached camera. The results obtained showed that nickel and tin modified the structure of the studied alloy and therefore altered the mechanical properties.

**NP 08**

**Synthesis of Platinum nanoparticles by Gamma radiolysis**

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The demand for polymers with intricate architecture expands with the advent of new applications using these materials, thus, leading to the discovery of novel methods for their production. Although the field of polymer synthesis has been extremely active, very few methods have been applied in industries due to their complexity and stringent requirements. We demonstrate the application of solvated electrons for rapid and selective polymerization of commercially available monomers at room temperature. The mechanism involving this method has been largely misunderstood due to an overgeneralized assumption made in the past. We first verify the inconsistent reports in literature regarding monomer selectivity and then provide evidence for a bi-mechanistic polymerization via radical anions. We show that the skewness of the molecular weight distribution can be employed to track initiation rate, which is crucial for the survival of the radical anions. This method is then further employed as a straightforward approach for producing block copolymers. |
The multi-functional Platinum Group Metals (PGMs) pure and hybrid nanostructures are based on a biomimicking approach. Marine organisms like diatoms and radiolaria provide materials scientists with many examples microstructures are formed by biomineralization a templated self-assembly process in which pre-organized organic surfaces regulate the nucleation, growth, morphology and orientation of inorganic crystals. Recently, various synthetic pathways that mimic aspects of biomineralization have been explored to produce patterned ceramic materials, among which the so-called EISA and EISA templating processes. This research project focuses on the development of pure and hybrid advanced 1-, 2- and/or 3-dimensional PGMs nano-composites for multi-functional technological applications by a versatile novel hybrid nanotechnology-nuclear process: Radiolysis and Evaporation Induced Self Assembly (EISA). The 0.1 M Pt solution of different concentration was prepared from K₂PtCl₄. The findings show the effect of irradiation on Pt II solutions with different concentrations irradiated at a certain dose. The UV-Vis spectrum of Pt of different concentrations shows a strong absorption peak at the wavelength 261 nm after irradiation, which indicates the presence of platinum nanoparticles. Furthermore, FTIR, XRD and HRTEM images also confirmed the presence of the nanoparticles produced by Radiolysis.

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<th>NP 09</th>
<th>Biosynthesis of magnesioferrite (MgFe₂O₄) nanocomposites by green method via Moringa Oleifera extract for electrochemical application</th>
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<tr>
<td>N. Matinise ¹, ², N. Mayedwa ¹, ², N. Mongwaketsi, M. Maaza ¹, ²</td>
<td>¹Nanosciences African Network (NANOAFNET) (iThemba LABS-National Research Foundation, Cape Town, South Africa) ²University of South Africa (UNESCO-UNISA Africa Chair in Nanosciences-Nanotechnology, College of Graduate Studies, Pretoria, South Africa). Email: <a href="mailto:nmatinise@tlabs.ac.za">nmatinise@tlabs.ac.za</a></td>
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<td>We present, for the first time, a novel magnesioferrite (MgFe₂O₄) nanocomposites bimetallic prepared by Green synthesis via Moringa Oleifera extract for electrochemical performance. Green synthetic route to produce an asymmetric electrochemical device using MgFe₂O₄ nanocomposites has not been published before. Green chemistry routes are on the rise due to their various advantages including cost effectiveness, no requirement of additional chemicals, reliability and the fact that is a very easy, environmental friendly method with a minimum of waste generation. Moringa oleifera plant is reported as sources of bioactive compounds including antibacterial, antifungal activity, antitumor, antiepileptic, anti-inflammatory, anti-diabetic, anti-ulcer, antioxidant and cholesterol lowering. Every part of the plant contains minerals, source of protein, amino acids and vitamins. These bioactive compounds have been shown to serve as both reducing and stabilizing agents for the fabrication of metal/bimetallic oxides nanocomposites. Their electrochemical activity, crystalline structure, morphology, isothermal behavior and optical properties will be studied using various characterization techniques such as X-ray diffraction (XRD) and Energy Dispersive X-ray Spectroscopy (EDS) cyclic voltammetry (CV), galvanostatic charge–discharge (GCD) and electrochemical impedance spectroscopy (EIS) Fourier transform-infrared (FTIR), High Resolution Transmission Electron Microscopy (HRTEM), Differential scanning calorimetry/thermogravimetric analysis (DSC/TGA), Ultra-violet visible (UV-vis) and Photoluminescence (PL). The mechanism of MgFe₂O₄ nanocomposites formation via the reaction of the precursors and photochemical bioactive compounds will be presented.</td>
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<th>Dieletric properties of VO₂ thin films synthesized using PLD</th>
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<tr>
<td>N. Numan ¹, ², G. Gaumann ², Nicolas ³, M. Chaker ³, T. Feurer ³, M. Maaza ¹, ²</td>
<td>¹Nanoscience and Nanotechnology laboratories, Materials Research Department, iThemba LABS, P.O. Box 722</td>
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<td>We present, for the first time, a novel magnesioferrite (MgFe₂O₄) nanocomposites bimetallic prepared by Green synthesis via Moringa Oleifera extract for electrochemical performance. Green synthetic route to produce an asymmetric electrochemical device using MgFe₂O₄ nanocomposites has not been published before. Green chemistry routes are on the rise due to their various advantages including cost effectiveness, no requirement of additional chemicals, reliability and the fact that is a very easy, environmental friendly method with a minimum of waste generation. Moringa oleifera plant is reported as sources of bioactive compounds including antibacterial, antifungal activity, antitumor, antiepileptic, anti-inflammatory, anti-diabetic, anti-ulcer, antioxidant and cholesterol lowering. Every part of the plant contains minerals, source of protein, amino acids and vitamins. These bioactive compounds have been shown to serve as both reducing and stabilizing agents for the fabrication of metal/bimetallic oxides nanocomposites. Their electrochemical activity, crystalline structure, morphology, isothermal behavior and optical properties will be studied using various characterization techniques such as X-ray diffraction (XRD) and Energy Dispersive X-ray Spectroscopy (EDS) cyclic voltammetry (CV), galvanostatic charge–discharge (GCD) and electrochemical impedance spectroscopy (EIS) Fourier transform-infrared (FTIR), High Resolution Transmission Electron Microscopy (HRTEM), Differential scanning calorimetry/thermogravimetric analysis (DSC/TGA), Ultra-violet visible (UV-vis) and Photoluminescence (PL). The mechanism of MgFe₂O₄ nanocomposites formation via the reaction of the precursors and photochemical bioactive compounds will be presented.</td>
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Dielectric properties of vanadium dioxide (VO2) thin film samples on sapphire substrate were investigated. The samples were synthesized using pulsed laser deposition (PLD) technique to ensure production of high quality thin films. Sample properties and composition were determined by X-ray diffraction (XRD); and scanning electron microscopy (SEM). The XRD results showed that, the samples exhibited monoclinic phase VO2 (M). Transmission spectroscopy measurements of the VO2 thin films were performed across the metal-insulator transition and the optical properties (such as transmission and absorption coefficient), were determined both at temperatures below and above the phase transition temperature; in the visible and the near-infrared part of the electromagnetic spectrum. The transmittance of VO2 thin films was observed to be inversely proportional to the thickness-dependent in the visible range and ranges between 85% and 98% for the 10 nm-thick films. 30% and 80% for the 50 nm-thick films; 10% and 55%, for the 100 nm-thick films, and 2% and 30% for the 200 nm-thick films. It was observed however that, the thinner films have a small change between the insulator and metallic phases in the vicinity of the transition temperature. The absorption coefficient can be determined by taking the negative gradient (using Beers law) of the linear fit of the logarithm of transmission data, for wavelength (250 - 3300 nm).

**References**


NP 11  Peptide functionalized Gold nanorods for the selective induction of apoptosis in target cells
Miché Desline Meyer
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The selective induction of cell death in cancer cells is the desired therapeutic goal of anti-cancer treatment. Targeted nano-therapeutic agents are showing promise for the selective removal of cancer cells. In a previous study, we showed that gold nanoparticle spheres (AuNS) bi-functionalized with a pro-apoptotic peptide and a receptor targeting peptide can selectively induce apoptosis in cells that express the receptor. Several studies have demonstrated the application of gold nanorods (AuNR) for the treatment of cancer using photothermal therapy (PTT). In the current study, we investigate the use of AuNRs bi-functionalised with the same pro-apoptotic peptide and receptor targeting peptide for selective induction of apoptosis. AuNRs were synthesized by the seed-mediated growth method with cetyltrimethylammonium bromide (CTAB). The gold nanoparticles (AuNPs) were then stabilized and bi-functionalized with the peptides. Subsequently, the AuNPs were characterized by UV-vis spectroscopy, Transmission Electron Microscopy (TEM) and Zeta potential measurements. Human cancer cell cultures were exposed to the bi-functionalized AuNPs and the viability of the cells was evaluated using the water soluble tetrazolium (WST)-1 Cell Proliferation assay and the induction of apoptosis examined by flow cytometric analysis. This study supports our previous findings by showing that cancer cells that express the ligand for the targeting peptide can
be selectively eradicated through apoptosis; furthermore we've shown that cells that do not express the targeting receptor are not affected by the AuNPs.

**NP 12**

**The Synthesis and Characterization of Boron-Containing Multiwalled Carbon Nanotubes using an Fe-Co/CaCO$_3$ catalyst**

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Carbon-based nanomaterials can be effectively modified by doping them with boron atoms in order to specifically tailor their structural, electronic and chemical properties toward specific applications such as organic solar cells [1], catalysis [2], electrochemistry [3] and photovoltaics [4]. It is, therefore, of interest to develop new techniques to produce doped carbon nanotubes. Herein, we report the synthesis of boron-doped multiwalled carbon nanotubes (B-MWCNTs) formed in the temperature range 700-900 °C via a chemical vapour deposition method using Fe-Co/CaCO$_3$ as the catalyst, acetylene as the carbon precursor and trimethyl borate as boron (and carbon) sources. The effects of boron doping and pyrolysis temperature on the formation of B-MWCNTs were studied. The resulting materials were characterized by transmission electron microscopy (TEM), X-ray powder diffraction (XRD), thermogravimetric analysis (TGA), Brunauer-Emmett-Teller (BET), Raman Spectroscopy, and X-ray photoelectron spectroscopy (XPS). TEM analysis revealed that the nanotubes exhibit bamboo-like structures with rough surfaces and relatively uniform diameter. At high synthesis temperatures (> 800 °C) bulbous-shaped catalyst filled tubes as well as solid and core-shell carbon spheres with chain-like morphology were also formed along with B-MWCNTs. The synthesis temperature and the boron source played a key role in determining the structures of the products. The optimum temperature for the synthesis of the B-MWCNTs was found to be 800 °C (B = 1.6%, as determined by XPS analysis). The B-MWCNTs exhibited good thermal stability in air.

**NP 13**

**Degradation of Chromium from water/wastewater by TiO$_2$ nanoparticles**

M. Ali Ahmed

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Waste water treatment one of the challenges facing the world in the 21st century. The improvement in human living standards, a steady increase in the world population and industrialization have resulted in environmental pollution in air, water and soil. Chromium exists in the environment in two oxidation states, Cr(III) which is an essential human nutrient and Cr(VI) which is the most toxic form of the element. This work aims to develop simple and cost effective methods in degradation of hexavalent chromium from water/wastewater to less toxic and easy separated trivalent chromium. Degradation will be using nano-sized Titanium dioxide (TiO$_2$) which is very promising photocatalyst material through reduction of water, due to its good charge transfer properties and high stability under the UV light, and testing it ability of reduction under direct sunlight. TiO$_2$ nanoparticles are prepared by sol-gel method using titanium tetra-chloride as precursor, annealed for structure quality and then characterized by Fourier transform Infra Red (FTIR), X-Ray Diffraction (XRD), Scanning electron microscope (SEM), and Energy dispersive x-ray Fluorescence spectrometer (EDX). Characterization indicated formation of Ti-O bonds, particles of size 30 nm and Anatase structure. Effects on Cr(IV) concentration were studied under the parameters of acidic pH alone, adsorption of TiO$_2$ nanoparticles in dark and outdoor direct Sun light on prepared Cr(VI) solutions
treated with TiO$_2$ were investigated to test degradation to Cr(III) efficiency under these circumstances. Cr(VI) concentration was investigated using UV-Visible spectroscopy systems, prior and after treatment with TiO$_2$. Results showed that prepared nanoparticles played important role in decreasing concentration of Cr(VI) for all pHs.

**NP 14 Effects of particle size variation on magnetic property of chemically synthesized magnetite nanoparticles**

Ezenwafor, T.C$^{1,2}$, Obayemi J.D$^3$, Obibuzor, C.V$^4$, Daniyan, E$^4$, Umar M.A$^4$, Haruna, M.S$^4$, Soboyejo, W$^{1,2}$

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This study presents the effect of particle size on the magnetic property of the chemically synthesized magnetite nanoparticles from Iron (III) nitrate (Fe(NO$_3$)$_3$.9H$_2$O) and Ethylene glycol (HOCH$_2$CH$_2$OH). The sol gel process was controlled by varying the concentration of iron nitrates keeping other parameters; the ageing time, pH and the volume of ethylene glycol constant. The purity of synthesized Magnetite (Fe$_3$O$_4$) and its surface composition was investigated using Energy Dispersed X-ray Fluorimetry (EDXRF) and X-Ray Photoelectron Spectroscopy (XPS), while the structure of the nanoparticles was elucidated via X-ray diffraction. The particle size and shape were characterized using transmission electron microscope and ImageJ software. Finally, the effects of the particle sizes on the magnetic properties of the nanoparticles were studied using Vibrating Sample Magnetometer (VSM). The VSM result revealed that the magnetite nanoparticles synthesized were super paramagnetic and variation in the nanoparticles size affects the saturation magnetization and normalise remanence. The implications of the results are discussed for the design of magnetic nanoparticles for disease detection.

**NP 15 Inhibiting effects of Copper nanoparticles on the corrosion behavior of 2101 Duplex Stainless Steel in 0.5m H$_2$SO$_4$**

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Corrosion inhibitors are substances which when added in small amounts into an environment can protect metals from corroding. Inhibitors usually protect metals by adsorbing themselves to the substrate and thus provide protection through the formation of a passive layer. Nanotechnology has been reported to assist in corrosion remediation of steel by introducing nanoparticles. Nanoparticles properties differ from bulk material of the same composition. Nano particles extracts are very good materials for corrosion because of their high surface areas which allow them to function as corrosion inhibitors. Their small particle sizes often cause unique chemistries not observed in bulk materials. The copper nanoparticles were obtained from the extracts of potato plants which are organic materials. They are biodegradable, non-toxic and available. The use of agro waste extends the beneficial use of the plant by turning agro waste to wealth, improving municipal waste management and also alleviating corrosion at a reduced cost. The inhibitive properties of copper nanoparticles derived by extract of potato leaves, roots and stem on corrosion of 2101 duplex stainless steel in 0.5M H$_2$SO$_4$ solution were investigated by electrochemical methods. The extracts were characterized with Atomic Absorption Spectroscopy (AAS) and Fourier Transformed Infrared Spectroscopy (FTIR) analyses. Copper nanoparticles inhibited the corrosion of 2101 duplex stainless steel in 0.5M H$_2$SO$_4$. 
Graphenised immunosensor for ESAT-6 TB biomarker
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Tuberculosis (TB), a deadly disease second to HIV/AIDS, is a global health problem. This disease is known to arise in two states, as an active state and as a latent state. Diagnosis of active tuberculosis is tedious and requires expensive procedures since there is no recognizable method for the sole detection of active TB. The current diagnosis consists of chest X-ray and multiple sputum cultures used for acid-fast bacilli. The TB diagnosis of children is difficult which further complicates the diagnosis. Therefore a rapid, sensitive and specific diagnostic method is imperative for the detection of TB. In this work an electrochemical immunosensors was developed for the detection and quantification of the TB antigen, 6 kDa early secretory antigenic target (ESAT-6). The development of the immunosensors was constructed on glassy carbon electrodes using electroactive layers of graphene oxide (GO) modified with Silver (Ag) nanoparticles to achieve a high degree of homogeneity and integrity of the platform. The combination of the nanoparticles with graphene layers was responsible for the high degree of electron transfer and high biocompatibility to effectively achieve the immobilization of anti-ESAT-6 and thus the electrochemical detection which was achieved through both impedimetric and amperometric techniques. Additionally, the surface morphology of graphene oxide, silver nanoparticles and the resultant graphene oxide/silver composite was characterized using High-Resolution Transmission Electron Microscopy (HRTEM), High-Resolution Scanning Electron Microscopy (HRSEM) and Atomic Force Microscopy (AFM) indicating in particular that the composite is silver-graphene oxide (Go-Ag). The structural analysis of the composite was achieved using Fourier Transform Infra-Red Spectroscopy (FTIR), ultra-violet spectroscopy (Uv-vis) and Raman Spectroscopy. FTIR and Uv-vis have a band around 689 cm⁻¹(C-O-C which confirms the formation of the composite) and 350 nm (which is absorption band for the composite) respectively. Cyclic voltammetry (CV) analysis of the GO-Ag/anti-ESAT-6 immunosensor for the detection of ESAT-6 antigen shows two oxidation peaks at (1000 µA and 1500µA) and the reduction peak (-2100 µA).The peak at 2000µA indicates the presence of Ag while, the one at 500 µA indicates the presence of GO while the one at 1500 µA indicates the combination of anti-ESAT-6 and ESAT-6. Additionally, the EIS data of the immunosensor revealed a single-phase shift (Ø = 70°) at a frequency of 2 Hz which corresponds to a capacitive behavior of ESAT-6 antigen after detection using the sensor. This proves that nanomaterials with carbon active material can be used for the detection of pulmonary TB using a sputum ESAT-6 antibody/antigen.

Synthesis, Characterization and effects of AuNP generated H₂S donor on cowpea in responses to drought conditions
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Cowpea (Vigna unguiculata) is a vital African indigenous legume crop known for its ability to grow in marginal soils. It is a good calorie source and an excellent source of high quality protein. The climate change leads to erratic rainfall patterns worldwide. This has resulted in the eight of the nine South African provinces to be declared drought disaster zones (Essop, 2016). Although, there is drought mitigation in place, a growing population makes them impossible to maintain. Thus, it is vital to develop new crop varieties such as cowpea with enhanced resilience to climate change. This project investigated the effect of gold nanoparticles synthesized from a H₂S donor (GY4137) on the responses of cowpea to drought. It is postulated that, H₂S has the ability to improve plant tolerance
to drought and GYY4137 gold nanoparticles (AuNPs) should improve cowpea drought tolerance at lower doses of GYY4137 than when GYY4137 is used on its own. Short lived GYY4137 capped gold nanoparticles were successful synthesized and compared to the alternatives of citrate and amino acid-reduced gold nanoparticles. The nanoparticles were all fully characterized by using standard techniques. The gold nanoparticles were all tested for the H₂S donor properties on cowpea in responses to drought conditions. These results will be discussed.

NP 18  
**Degradation of organic dyes using complex metal oxide of Zn₂SnO₄–SnO₂ as nanocatalyst**  
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Nanostructured photocatalysts have been proposed as possible alternative to the conventional methods of water treatment due to their ability to completely remove toxic chemicals from industrial effluents. In the quest to further enhance the physical and chemical properties of photocatalysts, ternary complex oxide has come into limelight. Compared with simple binary oxides, ternary complex oxides (multication oxides) have more freedom to tune the materials’ chemical and physical properties by altering the compositions. They are chemically more stable, making them ideal for applications in places of extreme conditions. Zinc tin oxide-Zn₂SnO₄ (ZTO) is an n-type transparent conducting polymer with a band gap of 3.6 eV and electron mobility of 10 to 15 cm²V⁻¹S⁻¹. Similarly, SnO₂ is one of the most attractive n-type wide band gap semiconductors that possess many outstanding properties such as good electrical conductivity, high optical transmittance, thermal stability, and mechanical hardness. SnO₂ has a more positive conduction band edge than ZTO. It is, thus, a better electron acceptor than ZTO; making the pair good candidate for heterostructure photocatalyst. We report here, ZTO–SnO₂ nanocomposites synthesized by a two-step technique. This involved firstly the microwave synthesis of ZnSn(OH)₆ as precursors from the aqueous solution of different concentration ratio of SnCl₂ dihydrate to zinc acetate dihydrate: 2, 5, 10, 15, and 20% using glucose as reducing and stabilising agent, and then followed by calcination of the precursors at 800 and 1000 °C in air. The optical and structural properties of the nanocomposite were studied. The optical band gap of the nanocomposites was greater than 4.1 eV, with observed increase directly proportional to increase in the concentration of the precursor SnCl₂. This blue shift in the optical band gap was due to the quantum confinement effect. The nanocomposite exhibited high photocatalytic properties on all selected organic dyes.

NP 19  
**Improved Specificity and Signal-amplification in the Adsorptive Cathodic Stripping Voltammetric (AdCSV) Determination of Ni(II), Co(II) an Zn(II) at Disposable, Graphene-modified Pencil Graphite Electrodes (PGE)**  
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Graphene-based chemical sensors have been widely used in the electrochemical sensing of metal ions and have demonstrated high performance as a signal amplification technique. To date, however, its application in the metal analysis has been limited primarily to the anodic stripping voltammetric (ASV) approach. The influence of electrodeposited graphene inclusion on the voltammetric response of pencil graphite electrodes (PGE) and its ability to improve electrode sensitivity was studied by adsorptive stripping voltammetry (AdSV). AdSV offers a fast, simple, sensitive, low cost and green electroanalytical technique for the determination of trace concentrations of metal ions, in water samples, with low solubility in metallic films. This research demonstrates a novel electrochemically reduced graphene oxide (ERGO)/mercury film (HgF) nanocomposite modified PGE, prepared through successive electrochemical reduction of graphene oxide (GO) sheets and in-situ plated mercury film. The ERGO-PG-HgFE, in combination with dimethylglyoxime (DMG), Nioxime, and Morin and square-wave cathodic stripping voltammetry (SW-CSV), was evaluated towards the determination of Ni\textsuperscript{2+}, Co\textsuperscript{2+} and Zn\textsuperscript{2+} respectively.

A single-step electrode pre-concentration approach was employed for the in-situ Hg-film electroplating, metal-chelate complex formation and its non-electrolytic adsorption at −0.7 V for Ni\textsuperscript{2+} and Co\textsuperscript{2+} and −0.3V for Zn. The current response due to metal-complexing agent was studied as a function of experimental variables; deposition/accumulation potential, deposition/accumulation time, rotation speed, frequency and amplitude and carefully optimized for the determination of Nickel and Cobalt at low concentration levels (μg L\textsuperscript{-1}) in 0.1 M ammonium buffer solution (pH 9.4) and 0.1 M acetate buffer solution (pH=4.6) for Zinc. Reduction peak currents varied linearly over the range of 2 and 16 μg L\textsuperscript{-1} and 1-10 μgL\textsuperscript{-1} respectively, for the individual analysis of Ni\textsuperscript{2+} and Co\textsuperscript{2+} concentration. The recorded limit of detection and quantitation was found to be 0.120 ± 0.002 µgL\textsuperscript{-1} and 0.401 ± 0.007 µgL\textsuperscript{-1} respectively, for Ni\textsuperscript{2+} and 0.219 ± 0.003 µgL\textsuperscript{-1} for Co at an accumulation time of 120 s. The ERGO-PG-HgFE further demonstrated a highly selective stripping response toward Ni\textsuperscript{2+} and Co\textsuperscript{2+} determination. The validity of the developed graphene-based sensor and method in real laboratory tap water samples was evaluated. This electrode was found to be sensitive enough to detect metal ions in the tap water samples at the 0.2 µgL\textsuperscript{-1} level, well below WHO standards.

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**Continuous Fabrication of Cellulose Nanocrystal/PEGDA Hydrogel Fibers**

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Advances in hydrogel design are yielding new hydrogel materials with diverse macroscopic topological structures. Among these, hydrogel fibers have been considered as a new class of hydrogel material with unique spatiotemporal properties. In this study, based on the novel non-template dynamic-crosslinking-spinning (DCS) method which has been demonstrated for scalable fabrication of size-controllable hydrogel fibers from oligomers, the method involved the use of one-step production of nanocomposite hydrogel fiber with weakly-gelled nanoparticle/oligomer (cellulose nanocrystals/poly(ethylene glycol) diacrylate, CNC/PEGDA) dispersion, where the interparticle interactions between CNC dominate the rheological property. The weakly-gelled CNC/PEGDA dispersion exhibited viscoelastic and shear thinning behavior, where continuous and uniform CNC/PEGDA hydrogel fibers were successfully fabricated by controllable extrusion. The diameter and water retention of the fibers could be controlled by the CNC content and spinning parameters. In addition, mechanical properties of the fiber were found to increase in the presence of CNC. This novel nanocomposite hydrogel fiber material has the potential on the fields such as...
Synthesis and characterization of epoxy matrix nanocomposites reinforced with zinc oxide nanoparticles

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In this research, an investigation was carried out on the development and characterization of epoxy matrix nanocomposites reinforced with zinc oxide nanoparticles. This was aimed at developing low cost-high performance epoxy matrix nanocomposites for various engineering applications. The particle size and morphology of the zinc oxide (ZnO) 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). Epoxy matrix nanocomposite samples were developed using 0, 2, 4, 6, 8, 10 and 12 wt. % of ZnO nanoparticles by open cast method. Mechanical properties tests were carried out on the samples in accordance with ASTM standards. Results obtained show that Ultimate Tensile Strength (UTS), flexural strength and hardness of the nanocomposite samples increased progressively with increase in weight percentage of ZnO nanoparticles reinforcement up to 8 wt. % after which slight decrease in hardness, flexural strength and UTS values were observed for samples containing 10 wt. % and 12 wt. % of reinforcement. Also, similar trend was observed for impact strength results with nanocomposites sample containing 10 wt. % reinforcement exhibiting the highest impact strength value of 11.17 KJ/m after which slight decrease in impact strength value was observed for sample containing 12 wt. % of reinforcement. However, ductility of the nanocomposites samples decreased progressively as the weight percentage of reinforcement increase. Results obtained from microstructural examination of the nanocomposites samples show that the nanoparticles were well dispersion in the matrix.

Preparation and characterization of nanostructured Nickel doped zinc oxide (Ni:Zno) thin film for solar cell application

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Nanostructured Nickel doped Zinc Oxide thin films have been deposited on soda lime glass and indium tin oxide (ITO) coated glass slide coated substrates by chemical spray pyrolysis technique (CSP). The influence of the Ni doping on the surface morphological and optical and electrical properties of the thin films were investigated using SEM with EDX, uv-vis spectrophotometer, keithley source meter 2400 coupled with four point probe and the I-V measurement in dark for the purpose of fabricating cheap, high efficient and environmental friendly Optoelectronic devices such as solar cell, LED etc. Morphological studies revealed that the films were continuous and the particles were uniformly distributed across the substrate’s surface with crystal size decreases with the present of Ni dopant. EDX indicates that the presence of Zn and O of ZnO film and Ni, Zn and O in the Ni:ZnO film with little or no impurities. Optical analysis of Ni:ZnO thin films gave high optical absorption in the uv-visible region. The band gap obtained ranged from 3.05 eV to 3.15 eV with a good rectifying properties.
Photonic Bandgap Fiber performance in chemical sensing (Nano-Optics)
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Nanophotonics is a new field of nano-science that deals with the interaction of light with matter on a micro/nanometer size scale. It is a field in which photonics merges with nanoscience and nanotechnology. This has spawned new areas of research for fiber optics and when we think of optical fibers, we typically think of optical propagation through waveguides of dimensions greater than or similar to the optical wavelength. Unlike conventional optical fibers, photonic bandgap fibers (a category of Photonic Crystal Fibers) do not guide light by total internal reflection but rely on a photonic bandgap in the fiber’s cladding. In a close analogy to the electronic bandgap in a semiconductor, a photonic bandgap occurs in a periodic optical material when the periodicity prohibits solutions to Maxwell’s equations for certain wavelengths. A photonic bandgap fiber consists of a hollow core surrounded by a cladding whose periodicity creates a bandgap for the photons guided in the fiber’s core. Photonic bandgap fibers are of intense interest for telecom applications because their optical characteristics - e.g., birefringence and dispersion -- can be tailored readily by fiber design, and because they have the potential to have lower loss than conventional glass fiber. The ~0.15-dB/km loss in conventional fiber cannot get much lower because it is caused by fundamental processes: Rayleigh scattering at short wavelengths and multiphoton absorption at long wavelengths. These losses become trivial in a photonic bandgap fiber because most of the optical power propagates in air, not in glass.

Usually, little attention need be given to sub-wavelength or nanometer size features. However, when nano-features are intentionally incorporated into optical fibers, many interesting phenomena may arise. For example, with nano-features of sufficient refractive index contrast, a properly designed optical fiber can do more than simply guide light from one point to another. Such features can be used to create different types of wave guiding phenomena as well as enabling capabilities for manipulation of light that go beyond conventional optical transport. This additional functionality offers great potential of fiber-based nanotechnology for applications in communications, computation, sensing, biology and chemistry for both waveguides and waveguide-based devices. The sensing mechanism takes place by detecting the analytes filled holes in the core region with the evanescent field through the interaction of lights. A proposal is made which shows high birefringence lower confinement loss and also shows high sensitivity for three analytes benzene, water and ethanol. A circular PBF is also proposed to make a comparative analysis with the proposed PBF.

Novel scheme for the production of nanosilica from non-returnable beverage bottles: an environmental pollution control perspective
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The emergence of non-returnable beverage bottles has led to serious environmental pollution problems because of the lack of a proper disposal system of used bottles. Common beverage bottles come in the form of beer bottles popularly known as ‘dumpies’ such as Castle Lite, Cider brands such as Savanna dry, Hunters Dry and other non-alcoholic bottles. We hereby report a novel strategy of containing pollution challenges associated with non-returnable beverage bottles. A high value material, nanosilica has been successfully synthesized from waste bottles using the sol-gel method. Characterization was done using powder XRD for structural analysis, UV-VIS Spectroscopy for absorption studies, FTIR for chemical structure analysis, FESEM for surface morphology and EDS for elemental analysis. It was found out that approximately 72% of nanosilica can be obtained per given weight of waste bottles. This study points to huge potential of economically recovering nanosilica by the proposed process for a myriad of applications such as nanopaint, cement, tire and plastics manufacturing. Incorporation of nanosilica as an additive to conventional materials can lead to high value composite nanostructured products.

NP 25 Control of Self-Polarization in PZT 50/50 thin films
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A number of mechanisms controlling self-poling in PZT thin films have been suggested in the literature. However, besides the role of interface polarity, no detailed work has been reported on the control of self-poling through manipulation of bulk properties in monocrystalline films. In this work we report systematic study of controlling self-poling through the use of use of different dopants and changing of stoichiometry (with excess PbO). The upward polarization of as-grown PZT thin films with strontium ruthenate (SRO) bottom electrode can be controlled to switch downwards through substrate with polar surface termination, using 25% excess PbO in the PLD targets, as well as doping. While interfacial mechanism seems to get weaker with film thickness, bulk work function modification through Nb doping appeared to play significant role in films as thick as 150 nm.

Figure: Undoped PZT 50/50 with 15% excess PbO on SRO. (a) AFM (b) PFM amplitude and (c) PFM phase. As grown film has upward polarization direction.

NP 26 Solar photocatalytic hydrogen production via Glycerol Reforming over transition metals supported TiO2 hollow spheres: preparation, characterization and photoactivity
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Nanostructured TiO$_2$ hollow spheres (THS) were prepared via a simple hydrothermal method with titanium butoxide, ethanol, urea, and ammonium sulphate. Transition metals such as Ni, Cr, Co, Ag, Cu were subsequently loaded on the surface of the THS using impregnation technique; and subsequently calcined in poor H$_2$/N$_2$ gas mixture at 450 °C for 4 hrs. The prepared photocatalysts were characterized using Brunauer-Emmett-Teller (BET), X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Photoluminescence (PL), and UV/vis. The SEM and TEM images confirmed the formation of uniform THS with large surface area; the XRD analysis revealed that the crystal phase structure of the THS particles was 100% anatase; and the DRS spectra showed that the doping THS with transition metals resulted in the reduction of the band gap. PL analysis also revealed that transition metal doping lead to a decrease in the rate of electron/hole pair recombination. The improved hydrogen evolution from photocatalytic reforming of glycerol was attributed to: the high surface area which enhanced the adsorption of glycerol onto the surface of photocatalysts; high crystallinity and the reduced band gap which improved the solar light harvesting; the hollow chamber within the TiO$_2$ spheres which produced multiple reflection of the light harvested, thus producing efficient electron/hole pair formation, and the detailed composition of the solids retarded the electron/hole recombination by trapping the electrons generated during the photo excitation of the photocatalysts, and thereby promoted their activity.
Synthesis of highly dispersed polymeric materials and application on wastewater remediation

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Nowadays, heavy metals and organic compounds are used in various processes such as metal coating of paints, electroplating, surface treatment, photography, electronics, etc. Congo Red (CR)[1-naphthalene sulfonic acid, 3.30-(4.40-biphenylenebis (azo)) bis (4-amino-) disodium salt] is a typical and the first synthetic dye of anionic azo dyes used in cellulose industries such as paper, pulp and cotton textile in the tropical zone. Cadmium [Cd (II)], one of three heavy metals and CR are serious hazard to aquatic living organisms and can cause carcinogen to humans. Due to the large discharged volume and effluent combustion, wastewaters are rated as the most polluting species among all industrial discharges. Their presence in water, even at very low concentrations, is distinctly visible; it is undesirable and may dramatically affect the photosynthetic activity in the aquatic life due to the reduced light penetration. In view of these reasons, the present study is focused on the bioanalysis of CR and Cd (II) removal from wastewater. The polymeric material highly dispersed on alginate and oxide of iron/aluminum were synthesized based on wood sawdust and orange skin wastes. The characterization of the synthesized materials by FTIR spectroscopic confirmed the withdrawal of extractibles, hemicelluloses and celluloses during the synthesis.

The removal of Cd (II) ions from synthetic wastewater by using alginate wood sawdust (Triplochiton scleroxylon) were investigated with respect to the adsorption parameters. The equilibrium data were modelled using Langmuir isotherm suggesting the monolayer adsorption of the cadmium. From D-R isotherm model, the mean free energy was calculated to be 5.39 kJ/mol, which indicated that Cd (II) adsorption ions could include an important physisorption stage. The highly dispersed polymeric materials were used as an electrochemical material for the preparation of carbon paste electrodes (CPE) named CPE-Fe, CPE-Al and CPE-Fe/Al, for iron, aluminum and mixed of iron/aluminum respectively, and were used as a working electrode for the electroanalysis of Congo Red (CR) in an aqueous medium. Two electrochemical techniques namely cyclic voltammetry and square wave voltammetry were operated for the bioanalysis of anionic dyes from wastewater. The obtained results have shown by cyclic voltammetry the reversibility of the system and the electronic transfer process of the analyte to the surface of the sensor was controlled by the diffusion. These values indicated that this electrode was very effective for the detection of Congo Red in synthetic wastewaters. The results indicated that the highly dispersed polymeric materials could be an alternative material in place of more costly adsorbents used for the wastewater remediation.

Secondary treatment of Macadamia activated carbon by sulphuric acid and phosphoric acid for improved Cr(Vi) adsorption from aqueous solution

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Cr(III) is an essential micronutrient found to be active in biological processes including glucose metabolism in mammals. In contrast, Cr(VI) is a carcinogen and is toxic to living organisms. Among various treatment technologies available, the most commonly used ones for the sequestration of chromium(VI) compounds from wastewater are the adsorption methods by synthetic polymers and by activated carbons derived from plant based materials. Adsorption methods offer economical and efficient platform for the removal of heavy metal pollutants including Cr(VI). Activated carbon adsorbents are known for their large surface area and abundant adsorption sites.

WP 01

WP 02
on the surface. In this study, *Macadamia* activated carbon (MAC) was refluxed under different concentrations of sulphuric acid and phosphoric acid in order to improve the structural characteristics of the adsorbent for improved Cr(VI) removal. Alteration of surface characteristics was confirmed by Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM) and thermogravimetric analysis (TGA). These techniques revealed that the acid treatment modified the surface properties of the adsorbent by imparting more oxygenated functional groups. Adsorption of Cr(VI) was carried out by varying parameters such as contact time, pH, concentration and adsorbent dosage. The optimum conditions for the adsorption of Cr(VI) were found at pH 1, contact time 12 hours, adsorbent mass 0.5 g and Cr(VI) concentration 25 mg/L. The results showed that treated MAC performed better than untreated MAC, signifying the effect of secondary treatment on enhanced removal of pollutants.

**WP 03**  
**Adsorptive performance of Banana peels nanosorbent in the removal of radioactive minerals from real mine water**  
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Transformation of agricultural waste such as banana peels into a valuable sorbent material has been proven effective and efficient in wastewater treatment. Further, transformation into nanosorbent to enhance the removal capacity of actinides (uranium and thorium) from mine water is extensively investigated in this study. The nanosorbent samples before and after adsorption were characterized by X-ray diffraction (XRD), Fourier transform infra-red (FTIR), while the amount of radioactive substances adsorbed was determined by inductively coupled plasma optical emission spectroscopy. Results revealed that there was a crystallite size and particle size reduction from 108 to 12 nm and <65,000 nm to <25 nm, respectively, as a function of milling time. The functional groups responsible for the banana peels capability to coordinate and remove metal ions were identified at absorption bands of 1730cm\(^{-1}\) (carboxylic groups) and 889cm\(^{-1}\) (amine groups) via FTIR analysis. Equilibrium isotherm model demonstrated that the Langmuir maximum adsorption capacity was 27.1 mgg\(^{-1}\) for uranium and 45.5 mgg\(^{-1}\) for thorium in synthetic water. Treatment of mine water revealed that the banana peels nanoadsorbent has good affinity for Th, U and other minerals present in mine water samples (Fe, As, Mo, Mn, Cd, Te and Bi). Consequently it can be concluded that nanostructured banana peels is a potential adsorbent for the removal of radioactive substances from aqueous solution and also from real mine water. However, the choice of this sorbent material for any application will depend on the water matrix to be treated.

**WP 04**  
**The synthesis and characterization of silver doped titanium dioxide nanoparticles and their photo-catalytic degradation of 2-chlorophenol**  
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Silver doped titanium dioxide nanoparticles have been synthesized in this study using different chemical methods. These materials were then characterized using Transmission Electron Microscopy (TEM), X-ray Diffraction (XRD), Fourier Transform Infra-Red Spectroscopy (FTIR), Ultra Violet Visible Spectroscopy UV-Vis and Thermal Gravimetric Analysis (TGA). In this study we also report the photo-catalytic degradation of 2-chlorophenol (2-CP) with the silver doped titanium dioxide nanoparticles. The TEM and XRD results showed the presence of Ag and Ti in the nanoparticles. The Ag and Ti were found to be well dispersed on the morphology of nanoparticles. TEM also showed that the particles were in the nanosize range (1 – 100 nm). FTIR and UV-Vis Spectroscopy showed the different absorption band and peaks of the nanoparticles. Results obtained revealed that Ag-doped TiO\(_2\) showed high activity for UV-photo-catalytic degradation of
2-CP. The photo-degradation follows a pseudo-first-order reaction and the observed rate constant values change with the 2-CP concentration. The presence of Ag ions in the TiO\textsubscript{2} structure caused a significant absorption shift towards the visible region. The photo-degradation efficiency matched the maximum light absorption efficiency.

WP 05 Preparation of V\textsubscript{2}O\textsubscript{5}-ZnO-coated carbon nanofibers: Application for removal of selected antibiotics in environmental matrices
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The removal of enoxacin and cinoxacin antibiotics from wastewater was investigated using V\textsubscript{2}O\textsubscript{5}-ZnO-coated carbon nanofibers as an adsorbent. The V\textsubscript{2}O\textsubscript{5}-ZnO-coated carbon nanofibers (V\textsubscript{2}O\textsubscript{5}-ZnO@CNF) nanocomposite was prepared and characterized using TEM, FTIR, PL, UV-Vis, SEM/EDX and XRD. The characterization results revealed that the V\textsubscript{2}O\textsubscript{5}-ZnO nanoparticles were incorporated on the surface of carbon nanofibers. The results obtained showed that the V\textsubscript{2}O\textsubscript{5}-ZnO@CNF nanocomposite had a better adsorption performance compared to V\textsubscript{2}O\textsubscript{5}-ZnO NPs and CNF. The effects of different experimental parameters such as adsorbent amounts, contact time, initial pH, that affect the removal process were optimized using Box-Behnken design. Under optimized conditions, the maximum adsorption capacity was found to be 112 and 96.7 mg g\textsuperscript{-1} for enoxacin and cinoxacin, respectively. In addition, the adsorption isotherms, kinetics and thermodynamics were used to investigate the adsorption kinetics.

WP 06 Synthesis of Lanthanum and Zinc terephthalic acid metal-organic framework and study of their methylene blue adsorption properties
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In this project, metal-organic frameworks (MOFs) of Lanthanum-benzene dicarboxylate (La(BDC)) and Zinc-benzene dicarboxylate (Zn(BDC)) were synthesized, characterized and studied as adsorbent for methylene blue removal in aqueous solution. Characterization of the La-MOF and Zn-MOF were carried out using Scanning Electron Microscopy (SEM), Brunauer-Emmett-Teller (BET) analysis, Energy-dispersive X-ray Spectroscopy (EDX), X-Ray Diffraction Analysis (XRD), Thermogravimetric Analysis (TGA) and Fourier transform Infrared Spectroscopy (FTIR). The removal of methylene blue from aqueous solutions varied with concentration, contact time and temperature. All adsorption studies were carried out in batch experiments.

WP 07 Removal of hexavalent chromium from aqueous solution using amino modified Macadamia powder nutshells
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Agricultural waste such as Macadamia nutshells are currently receiving more attention for removal of hexavalent chromium (Cr(VI)). However, they have low adsorption capacity when used in their raw form. In this study, the efficiency of using Macadamia nutshell powder modified with different concentrations of hydrogen peroxide, grafted with amino groups (diphenylcarbazide) for the removal of hexavalent chromium from aqueous solution was explored. The effects of various parameters controlling the adsorption of Cr(VI) onto Macadamia adsorbents such as initial
concentration, contact time, adsorbent dosage and pH were investigated. The optimum operating parameters were determined to be 150 mg/L, 3 h, 0.1 g and pH 3, respectively. Fourier transform infrared (FTIR) spectroscopy of the adsorbents revealed that treated material showed more carbonyl groups, while untreated (raw) *Macadamia* lacked such groups. Scanning electron microscope (SEM) showed that the treated material extracted more pores on the surface of the treated adsorbent allowing the diphenylcarbazide to be grafted more easily for removal of Cr(VI). The results revealed that diphenylcarbazide treatment improved the removal efficiency of Cr(VI).

**WP 08**  
**Application of green synthesized silver nanoparticles: an environmentally benevolent approach in waste water treatment and catalytic activity of benzyl alcohol oxidation with hydrogen peroxide**  
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University of Namibia, Windhoek, Namibia  
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Metal nanoparticles are endowed with optical, electrical and chemical properties. Among them, silver nanoparticles have unique distinctive biological and physico-chemical properties, including chemical stability, catalytic activity and antimicrobial properties. The aim of this study is to investigate the antimicrobial and catalytic properties of silver nanoparticles. Namibia is a semi-arid country in Southern Africa, and man-made dams play an important role in salvaging water. These dams are however periodically frequented by microalgae blooms that pose devastating effects on the water quality, making water treatment processes troublesome and cost prohibitive. On a different note, several noble metals such as Platinum, Titania, Gold and Palladium nanoparticle catalysts have been reported in literature with regard to the conversion of alcohols to aldehydes. Nevertheless, the attention received by silver nanoparticle catalyst for the oxidation of alcohols is very slow. An environmentally friendly protocol is being developed for synthesizing silver nanoparticles using a banana peel extract as both a reducing and stabilizing agent. Silver nanoparticles will form when the reaction conditions are altered with respect to pH, banana peel extract, concentration of silver nitrate and incubation temperature. UV–visible spectroscopy, Scanning Electron Microscope, X-ray Diffraction and Fourier transform infra-red spectroscopy will be used to characterise the silver nanoparticles formed. The antimicrobial activity of the silver nanoparticles will be tested to determine effectiveness for algal bloom inhibition in Windhoek waste water. Lastly catalytic properties of the silver nanoparticles will be tested by oxidation of benzyl alcohol to benzoaldehyde using 30% hydrogen peroxide. Percentage yield and purity will be determined.

**WP 09**  
**Synthesis and optimization of pine-magnetite composite for removal of methylene blue dye**  
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Purity and quality of water is a basic concern to mankind. The environment is deteriorating daily due to industrial pollution. Dyes discharged together with industrial textile wastewaters are main organic pollutants because they are highly visible and undesirable even at low concentrations in water. Natural biomaterials have been applied previously as adsorbents for dyes from aqueous solution, but their application has been limited by low adsorption capacity. In this study, pine cone biomass, a naturally occurring agricultural waste was treated with 0.15M NaOH solution to remove unwanted plant extracts and iron oxide magnetic particles was coated on the pine surface. The main focus of the study was to prepare and optimize the working conditions for the pine magnetite composite. The bio-nanocomposite material was synthesized by a complete co-precipitation method of Fe\(^{2+}\):Fe\(^{3+}\) (1:2) under alkaline conditions in an inert environment followed by addition of the biomass. The variables used for the experiments were volume of NH\(_4\)OH varied from 5ml to 40ml, reaction temperature varied from 40°C to 100°C and mass from 1.0g to 3.5g.
Incorporation of magnetite nanoparticles onto the surface of the biomass was confirmed by FTIR, TGA and XRD. TEM showed particles size ranging from 8.23 to 11.73. XRF showed the iron oxide content ranging from 57 to 74%.

**WP 10**

**Effects of nonlinear gradient terms on the defect turbulence regime in weakly dissipative systems**

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We investigate the behavior of traveling waves in a defect turbulence regime with the periodic boundary conditions by using the lowest-order complex Ginzburg-Landau equation (CGLE), and we show the effect of the nonlinear gradient terms in the system. It is found that the nonlinear gradient terms which appear at the same order as the quintic term can change the behavior of the wave patterns. The presence of the nonlinear gradient terms can cause major changes in the behavior of the solution. They can be considered like the stabilizing terms. The system which was initially unstable or chaotic can become stable by including the nonlinear gradient terms.

**WP 11**

**Synthesis and application of Cobalt 1,3,5-benzenetricarboxylate metal organic frameworks (Co-MOF) as adsorbents for the removal of toxic metal ions from aqueous solution**

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In this paper, we report the synthesis of metal organic framework of cobalt 1,3,5-benzenetricarboxylic acid (Co-MOF) by solvothermal method. The synthesized MOF materials were characterized by infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), (TEM), energy dispersive x-ray spectroscopy (EDX), thermogravimetric analysis (TGA) and Brunauer-Emmett-Teller (BET) analysis. Afterwards, the MOF materials were applied as adsorbents for the removal of toxic metal ions (Pb\textsuperscript{2+} and Cr\textsuperscript{3+}) from aqueous solutions. Various parameters were evaluated such as pH, initial metal concentration, reaction time, and adsorbent dosage.

**WP 12**

**Removal of 4-Nitrophenol using (Fe\textsubscript{3}O\textsubscript{4}) Nano-biocomposite crosslinked cyclodextrin from aqueous solution**

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Due to the toxicity and bio accumulative nature of organic pollutants, numerous approach for the treatment of contaminated waters have been explored. The study aimed to develop a cyclodextrin-magnetite nano-biocomposite for the removal of 4-Nitrophenol from aqueous solution. The magnetic nano-biocomposite (Fe\textsubscript{3}O\textsubscript{4}-PCP) material was synthesized by incorporating magnetite onto pine cone powder by co-precipitation method. Cyclodextrin was then crosslinked onto the synthesized Fe\textsubscript{3}O\textsubscript{4}-PCP by hexamethylene diisocyanate. The morphology, composition, magnetic properties and thermal stability of the composite was characterized using TEM, FTIR,
VSM and TGA/DTA analysis. Batch adsorption experiment such as effect of solution pH and adsorbent dose were conducted. Kinetic studies were carried out in batch reactions using various 4-nitrophenol initial concentrations (25-150 mg/dm$^3$). Successful cross-linking of cyclodextrin onto the surface of Fe$_3$O$_4$-PCP was confirmed by FTIR, VSM, TEM and TGA. The results revealed that the highest adsorption capacity of 23.40 mg/g was observed at optimum solution pH of 7 and adsorbent dose of 0.1 g for the adsorption of 4-Nitrophenol from CD-Fe$_3$O$_4$-PCP material after 2 hours of contact. Pseudo second order model well describes the kinetic data since the modelled capacity was close to the experimental capacity. The adsorption of 4-Nitrophenol onto magnetite-biomass was controlled by chemisorption.

**WP 13**

**Application of activated carbon decorated polyacrylonitrile nanofibers as an adsorbent in dispersive solid phase extraction of fluoroquinolones in wastewater**

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A simultaneous preconcentration method for ciprofloxacin (CIPRO), danofloxacin (DANO) and enrofloxacin (ENRO) in wastewater samples and the determination by high performance liquid chromatography was developed. The dispersive solid phase extraction method was based on the extraction of the selected fluoroquinolone antibiotics using tyre based activated carbon decorated polyacrylonitrile (PAN) nanofibers as an adsorbent. Optimization of influential experimental parameters such as pH, mass of adsorbent, extraction volume and extraction time was performed using small central composite design. The developed method presented limits of detection of 0.05, 0.11 and 0.20 µg L$^{-1}$ and limits of quantification of 0.17, 0.37 and 0.67 µg L$^{-1}$ for CIPRO, DANO and ENRO, respectively. The precision of the method was determined in terms of repeatability (intraday, n = 20) and reproducibility (interday, n = 5). In addition, an excellent linearity was achieved in the range of 500 - 1 µg L$^{-1}$, LOQ (R$^2$ = 0.998) at a preconcentration factor of 15. The intraday and interday precision reported in terms of the percentage relative standard deviation was 3% and 4%, respectively. The accuracy of the DSPE was validated by spike recovery tests, and results proved the reliability and efficiency in adsorbing antibiotics in wastewater. The recoveries of all antibiotics were satisfactory and were in a range of 98-102%. Finally, the proposed method was applied in wastewater samples collected from the wastewater treatment plant which includes influent, secondary and effluent wastewater. The proposed method was rapid, easy to use, and small consumption of organic solvent for the detection and determination of trace levels of antibiotics in environmental waters.

**WP 14**

**Adsorption of benzene from aqueous solution using acid coated magnetite nanoparticle**

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Contamination of aquatic systems by synthetic organic contaminants and emerging pollutants poses significant public and environmental health risks. The study aimed to coat the magnetite nanoparticle with oleic acid for the removal of benzene from aqueous solution. The magnetic nanocomposite (Fe$_3$O$_4$-OA) material was synthesized by the microwave method using ammonium hydroxide as precipitating agent. The morphology, functional groups and thermal stability of the nanomaterial was characterized using SEM, FTIR and TEM analysis. Batch adsorption experiment such as effect of solution pH, adsorbent dose and initial benzene concentration were optimized. The equilibrium adsorption data was then analyzed using the Langmuir and Freundlich isotherms
Coating of magnetite nanoparticles with oleic acid was confirmed by FTIR, SEM and TGA. The study also showed that the removal of benzene from aqueous solution is highly dependent on solution pH with optimum uptake achieved at solution pH of 7, adsorbent dose of 0.1g and optimum concentration of 250 mg/dm$^3$. The adsorption capacity of the biomaterial composite was 81.392 mg/g. The biomaterial composite has shown effectiveness for removal of benzene with adsorption while Langmuir isotherm gave a better fit of the equilibrium uptake of benzene from aqueous solution.

<table>
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<th>WP 15</th>
<th>Photocatalysis of methyl orange using Ag/AgCl catalyst under solar and LED light illumination</th>
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<td>John Akach$^1$, Frank Nembudani$^1$, Felistus Ramane$^1$, Aoyi Ochieng$^1$</td>
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<td>$^1$Vaal University of Technology (Centre for Renewable Energy and Water, Vanderbijlpark, South Africa)</td>
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<td>Email: <a href="mailto:johna@vut.ac.za">johna@vut.ac.za</a></td>
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Dyes from textile industries are major pollutants due to their strong colour and toxicity to aquatic life. As a result, several methods such as adsorption and advanced oxidation processes have been developed to remove them from wastewater. In this respect, photocatalysis has emerged as one of the best methods for textile wastewater decolorization. Conventional photocatalysis using TiO$_2$ is costly due to the high cost of UV light and catalyst separation. In this work, a visible light active Ag/AgCl catalyst was synthesized and applied for methyl orange decolourization. The optimum catalyst loading and effect of different light sources was investigated. It was found that the optimum catalyst loading was 0.3 and 0.2 g/L under solar and LED illumination, respectively. The rate of photocatalysis was found to be higher under solar than under LED illumination. This study showed that the Ag/AgCl catalyst could be used to effectively decolourize textile wastewater under solar illumination.

<table>
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<th>WP 16</th>
<th>Heterogeneous Fenton’s degradation of methylene blue by activated carbon-iron oxide composite: kinetics study &amp; mechanism</th>
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<tr>
<td></td>
<td>Kelebogile Mmelesi$^a$, Augustine Ofomaja$^a$ and Elvera Viljoen$^a$</td>
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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 [1]. 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 pseudo-first, 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 H$_2$O$_2$ 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 [2], 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.
| WP 17 | Production of Ceramic Pot Filters for Water Treatment Interventions Using Locally Sourced Materials  
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The need to improve on the flow rate and maintain the quality of the filtrate using ceramic pot filter so as to improve the access to potable water in the rural areas informed this work. Mixtures of clay, diatomite and sawdust were utilized in the production of ceramic pot filters. The percentage mixtures were as follows; A (sawdust 65, clay 25, diatomite 10) B (sawdust 60, clay 25, diatomite 15), C (Sawdust 50, clay 25 diatomite 25) and D (sawdust 45, clay 25, Diatomite 30). Physical and chemical analyses of the clay and compounded mixtures were done and result confirmed the suitability of the materials for the production of ceramic water filter pots. Solid casting method was used in the production and the produced water filter pots which were further coated with silver solutions were utilized in filtering water samples from a rural community. Results show that sample A gave the best results in terms of flow rate and removal efficiency. This implies that the inherent problems of water borne diseases prevalent in rural communities due to inaccessibility to supply of good quality and clean water could be solved. |
| WP 18 | Direct synthesis and characterization of cysteine-capped water soluble copper selenide quantum dots  
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Copper chalcogenide nanoparticles (NPs) have gained particular interest in electronic applications due to their unique optical and electrical properties. Copper chalcogenide nanoparticles are p-type semiconductors and are widely used to make hetero-junctions in solar cell devices. Synthetic methods for high-quality monodispersed nanoparticles in organic solvents are well-developed, but their biological applications are restricted due to the lack of water solubility and tailored surface chemistry. Herein we report on the synthesis of water soluble nanocrystals of CuSe via the direct use of hydrophilic ligand. We further report on the optical and morphological properties of CuSe nanoparticles as a function of temperature. The employed synthetic method successfully yielded water soluble CuSe nanoparticles with a single crystal phase. However, the morphologies of the cysteine-capped nanocrystals showed a well-define spherical and elongated nanorod like morphology of nanoparticles that are monodispersed. The synthesized CuSe nanoparticles were characterized using ultraviolet spectroscopy (UV-Vis), fourier transform infrared (FTIR), photoluminescence (PL), to determine the optical properties, transmission electron microscopy (TEM) to determine the particle morphology, and X-ray diffraction (XRD) to reveal the crystalline nature of the nanoparticle. |
| WP 19 | Synthesis, characterisation and assessment of antimicrobial activity of doped zinc oxide nanoparticles against selected waterborne pathogens  
N.E. Volofu¹, M.J. Klink¹, N. Laloo² and F. Mtunzi³  
Faculty of Applied and Computer Sciences, Department of Biotechnology¹, Chemistry², Vaal University of Technology, Private Bag X021, Vanderbijl Park, 1900, South Africa  
Email: nevolofu@gmail.com |
Clean water is a basic necessity for human life. Presently, most of the natural water reservoirs are significantly contaminated with pathogenic microorganisms. Therefore, there is a necessity to develop an effective antimicrobial agent to control growth of microbial population. Nanotechnology offers a way to develop new inorganic antimicrobial agents. The purpose of this study is to synthesise and characterise Cobalt oxide (CoO), Zinc oxide (ZnO) and doped ZnO nanoparticles and assessment of their antimicrobial activities against waterborne pathogenic yeasts, moulds, protozoa, fungi and bacteria. ZnO nanoparticles were synthesized using urea-based method at four different ratios. The precipitate was white. CoO nanoparticles were prepared at five different ratios using Cobalt nitrate and ammonium carbonate as the starting materials. The product was pink and became black due to calcination. Antimicrobial activity was assessed using minimal inhibitory concentration (MIC). Working concentration of the nanoparticles was 2 mg/ml. CoO nanoparticles did not inhibit growth against *Salmonella sonnei* and *Staphylococcus aureus* at this concentration. ZnO nanoparticles inhibited growth of these organisms at a concentration (MIC) of 12, 5 and 6.25 µg/ml, depending on the ratio.

WP 20

**Studies for Use of Reclaimed Water for Construction Industry in Maputo, Mozambique**  
Noor Jehan Gulamussen, André Marques Arsénio, Louis Cornelis Rietveld  
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The use of reclaimed water for non-potable uses is encouraged in situations where the demand of water is higher than the available water, as the case of Maputo, the capital of Mozambique. Drinking water is commonly used for concrete production, but previous experiments worldwide have shown the possibility of using non-potable water. The effluent from wastewater treatment plant in Maputo was found to comply for the most important quality parameters with the requirements for concrete production except for ammonium and foam vanishing time. Since most of detergents have phosphate in their composition, the vanishing time can be associated with the presence of phosphate. In this work, the influence of ammonium and phosphate in the quality of concrete blocks is investigated at pilot scale in a construction company. Drinking water spiked with ammonium and phosphate in same concentrations as found in treated wastewater was used to produce concrete blocks and then tested the resistance to compression on the 3rd, 7th and 14th days of cure and compared with drinking water and disinfected treated wastewater. Additionally water absorption was determined, and the morphology was evaluated by scanning electron microscopy. The 14th day results of the strength show that for all tests the values are below the limit except for chlorinated wastewater and drinking water. From water absorption tests apparently there is no link between the strength and the presence of ammonium and phosphate which is confirmed by the SEM images. In conclusion, the effluent from wastewater treatment plant can be used for concrete production with addition of chlorine or have to be post treated to remove the ammonium and phosphate.

WP 21

**Study of the adsorption capacity of Cu^{2+}, Fe^{2+} and Zn^{2+} in water by banana and orange peels as biosorbents**  
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Banana and orange peels are materials that have shown to have capacity to adsorb heavy metals. In Mozambique this material are abundant and usually are wasted after the use of fruits. In this study, the sorption capacity of banana and orange peels was investigated for removal of Cu, Fe and Zn in water. Sorption tests were carried out varying the granulometry, the amount of biosorbent, the contact time between the sorbent and adsorbate, the pH and pyrolysis temperature of the biomass, in order to determine the optimum conditions for better efficiency.
The biosorbents were characterized by scanning electron microscopy, where a highly porous, permeable, irregular, fibrous, spongy, rugose and heterogeneous structure was observed in both biosorbents, which are probably the aspects that facilitate the adsorption of heavy metals in water. The variation of particle size showed that the adsorption rate decreased from 77.9%, 79.7% and 85.4% to 19.9%, 31.8% and 33.2% for Cu, Fe and Zn respectively, when the particle size increased from 0.335 mm to 5.66 mm. The amount of biosorbents required for the adsorption equilibrium were 1.5, 1.0 and 3.0 g for Cu, Fe and Zn, respectively. The minimum time required to reach the maximum adsorption peak varied from 15 - 30 min for banana, orange and mixture of banana and orange peels, above that interval the adsorption process remained almost constant. The pH of 5 was ideal for removal of all metal ions. The pyrolysed shells at 200°C showed better adsorption efficiency, where the highest adsorption of 95.8%, 96.5% and 98.5% was obtained for Cu, Fe and Zn respectively. In the study of adsorption of referred metals from Revue river water was tested and removal efficiency’s of 64.2%, 55.5% and 73.8% for Cu, Fe and Zn respectively, could be reached with the optimum conditions.

WP 22
Selective sample preparation based on imprinted polymers, accurate profiling and generation of baseline studies of boating pollution in the Okavango Delta
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In this study accurate profiling of boating pollution in the Okavango Delta was conducted for the first time employing novel imprinted polymers coupled to either dispersive liquid-liquid micro-extraction gas chromatography mass spectrometry (MIP-DLLME-GC-MS) for the analysis of traces of suspected organic boating pollutants from fuels or coupled to microwave assisted extraction micro-plasma atomic emission spectroscopy (MIP-MAE-MPAES) for the analysis of suspected traces of heavy metals from paints used to coat the bodies of boats. The Okavango delta is the largest inland delta and it’s famous for its pristine waters and diverse natural flora and fauna. In the recent past, owing to its fame, the Okavango Delta has experienced increased tourism, including recreational boating activities. Increase of tourism activities has possibly led to increased boating pollution of the surface waters. It is on this backdrop that it was necessary to accurately profile for boating pollution, provide for the first time baseline studies of boating pollutants in the Okavango Delta and perform continued monitoring in the future. Thus, water and sediment samples were collected form areas with major boating activities; from the panhandle upstream (Shakawe) to downstream Matlapeng in Maun, Botswana. The pH of water was found to be relatively neutral, ranging from 7.08 to 7.64 with mean electrical conductivities between 46.3 μScm⁻¹ upstream (Shakawe) and 107.3 μScm⁻¹ in Matlapeng. Mean dissolved oxygen values ranged from 4.1 to 5.9 mgL⁻¹. Pollutants such as toluene, n-benzenes, xylenes, naphthalene, dodecane and cyclopentane were detected in water and sediment samples (not quantified yet). The concentration of heavy metals commonly added in boat paints such as zinc, manganese, lead, copper and cadmium were found to be ≤0.0540 ± 0.0030, ≤0.0507 ± 0.0051, ≤0.02125 ± 0.0012, ≤0.06333 ± 0.0033 and ≤0.01788 ± 0.0017 mgL⁻¹ respectively at n=3.

WP 23
Photocatalytic Degradation of a textile dye using Ag₃PO₄/Nanocellulose Composite
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Photocatalysis is currently considered an environmental-friendly and advanced technology for degradation of organic matter, which includes organic dyes from industrial wastes and pharmaceutical residues from the environment. For efficient degradation of organic matter,
Photocatalysts with high energy conversion material are highly sought out. Hence, the use of metal oxides with capability of exploiting visible light. Metal oxides catalysts can be stabilised by incorporation of certain polymers, for example cellulose; a cheap and sustainable biopolymer has been used to host different types of nanoparticles (NPs) to aid nanoparticle dispersion and consequently improve photocatalytic activities. Nanocellulose-based nanocomposites exhibit synergistic advantage offered by the combination of two nanomaterials. Nanocellulose (NC) offers intrinsic properties such as high porosity, mechanical strength as well as being good adsorbent for organic matter whereas Ag₃PO₄ NPs are high energy conversion material. We therefore fabricated and characterized an efficient visible light Ag₃PO₄ catalyst supported on NC films. Ag₃PO₄ NP/NC composite was prepared in situ by dispersing cellulose in a solution of Na₂HPO₄ in deionised water and ethylene glycol (1:3 (V/V)). AgNO₃ was then added to the cellulose mixture, which immediately turned yellow. The composite mixture was washed several times with water and characterized using XRD, SEM and TEM. The XRD results confirmed formation of Ag₃PO₄ while SEM and TEM showed spherical Ag₃PO₄ NPs well dispersed on nanocellulose sheets. The developed Ag₃PO₄ NPs/NC nanocomposite was applied in the degradation of methyl orange, an azo dye used in textile industry. The catalyst was able to completely decolourize methyl orange performed under solar irradiation within 2 hours in both deionised water and wastewater effluent. The results proved that nanocellulose is an excellent scaffold for Ag₃PO₄ NPs, making a composite catalyst that has potential to solve environmental pollution as well as challenges of energy supply through the use of solar energy.

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WP 24 Treatment of 50 000 litres per day of textile effluent using nanomembrane filtration: A Novel Approach of Improving Water Treatment
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Water pollution has rapidly increased over the past two decades. Water scarcity, high water costs, stricter regulations and need of supplementary sources of water to help fulfil future demands require more advanced water treatment technologies for industrial and urban water processes. According to Spiegler “the quest includes new unconventional sources of water such as the renovation and reuse of wastewater and desalination of brackish and sea water”. Several new unit processes for water and waste water treatment have been developed. These include the membrane process as a group, which can be divided into pressure –driven and electrically process. The textile industry utilizes various chemicals and large amount of water during the production process. About 200 L of water are used to produce 1 kg of textile. The water is mainly used for application of chemicals onto the fibres and rinsing of the final products. The waste water produced during this process contains large amount of dyes and chemicals containing trace metals such as Cr, As, Cu and Zn which are capable of harming the environment and human health. The textile waste water can cause haemorrhage, ulceration of skin, nausea, skin irritation and dermatitis. The chemicals present in the water block the sunlight and increase the biological oxygen demand thereby inhibiting photosynthesis and deoxygenation process. (Shannon MA, 2008). The membrane separation process is thought to be especially useful in water renovation because they allow separation of dissolved materials from one another or from a solvent, with no phase change. Therefore, introducing nano –membrane filtration for water purification is vital as it provides an attractive solution for cost-effective removal of contaminants with a small footprint. Nanomembrane filtration will get rid a wide spectrum of water contaminants due to its small pore diameters and also helps in chemical recovery which may reduce production costs.

WP 25 Chitosan nanofiber for removal of acidic pharmaceuticals from wastewater
Niragire H¹, Dube S¹, Maaza M²
The utilisation of chitosan as an adsorbent has attracted attention in the area of water treatment due to its special properties owing to amino and hydroxyl functional groups in its chemical composition. This research work assesses the capability of chitosan nanofibers as material for the removal of acidic drugs from wastewater. Nanofibers were obtained by electrospinning a blended solution of chitosan and polyvinyl alcohol (PVA). The blending ratio was optimized and nanofibers were successfully synthesized from 70/30 (PVA/chitosan) blending ratio. Nanofiber mats were then collected at optimum voltage of 20 kV, flow rate of 0.2 mL/h and tip-collector distance of 10 cm. The nanofibers had diameters of ca380 nm and were also characterised using SEM, FTIR, TGA-DSC and XRD. The percentage removal was found to be 64.6% (acetylsalicylic acid), 63% (naproxen), 62% (fenoprofen) and 100% (diclofenac) when using ultra-pure water spiked with these drugs. However, the percentage removal dropped to 40.8% (asa), 37.2% (naproxen), 59.0% (fenoprofen) and 60.6% (diclofenac) when the nanofibers were applied to wastewater. Maximum removal capacities ($q_m$) were calculated from Langmuir isotherm and were found to be 27.85 mg/g, 1666.66 mg/g, 166.6 mg/g and 1250 mg/g for acetyl salicylic acid, naproxen, fenoprofen, and diclofenac respectively. Equilibrium adsorption obeyed Langmuir and Freundlich isotherms. Langmuir was best fitting with correlation coefficient of 0.998 (asa), 0.993 (naproxen), 0.996 (fenoprofen) and 0.985 (diclofenac) indicating that the monolayer adsorption occurred on the surface on the nanofibers mats.
### Poster MP 01

**Laser-Induced Breakdown Spectroscopy (LIBS) on geological samples: quantification of relative hardness properties**

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This paper reports on the effects of LIBS experiment for quantification of relative hardness properties. The technique depends on the correlation between the intensity ratio of ionic to atomic spectral lines and the hardness of the target material. For generation of laser induced plasma, a Q-switched neodymium-yttrium aluminium garnet (Nd: YAG) laser operated at 10 Hz and wavelength of 1064 nm was employed on the surface of the samples. A spectrometer fitted with an intensified charge-coupled device (ICCD) was used to record the diffracted spectrum. The spectrometer was attached to a computer for rapid processing and interpretation of the data acquired. A Variety of samples was measured, the sample set was compiled from the samples collected directly from: (1) the Gold, Copper, and Iron mines in South Africa; (2) the Karoo (Prince Albert Formation (Fm) in South Africa; and (3) the Karas region in Namibia. To validate this method the results from the LIBS technique were correlated with subsequent analysis of the same samples by a mechanical technique, where the hardness number (HN) was used to estimate the hardness of these samples. Based on theory and results, LIBS is proposed as an analytical tool for estimation of relative hardness of geological samples.

### Poster MP 02

**An alternative low-cost adsorbent for gold recovery from cyanide-leached liquors: isotherm and kinetic studies**

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The focus of this research was to conduct a study in which activated carbons derived from waste Macadamia shells were used in the recovery of gold. These activated carbons (ACs) were modified with HNO\(_3\) and H\(_3\)PO\(_4\) to increase their surface adsorption properties and further explore if ACs produced from Macadamia nuts shells could be an attractive alternative or a complementary supplement to the coconut shell based carbons that are currently being used in the gold extraction industry in South Africa. The secondary modification of the Macadamia activated carbons was done with 3 different concentrations for both nitric acid and phosphoric acid. The modified activated carbons were labelled MACP\(_{20}\), MACP\(_{40}\), and MACP\(_{60}\), to signify the materials prepared from 20%, 40% and 60% (v/v) H\(_3\)PO\(_4\), respectively or MACN\(_{20}\), MACN\(_{40}\), and MACN\(_{55}\), to correspond to the three different concentrations of nitric acid used. Brunauer-Emmet-Teller, scanning electron microscopy, Fourier transform infrared spectroscopy, thermogravimetric analysis, elemental analysis and X-ray diffraction spectroscopy were used to characterize the prepared ACs. The physical properties were attained through determining attrition, ash content, volatile matter, and moisture content of all the activated carbons. Various
### MP 03

**Morphology of fractured surface of natural rubber–toughened polypropylene**  
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Polypropylene has poor low temperature impact resistance although it has a number of valuable properties. A well-established process for improving toughness and impact resistance in otherwise brittle polymers is by the incorporation of a dispersed rubber phase. The combination of an elastomer and a thermoplastic in one material generally leads to a two-phase, immiscible and incompatible material and often requires a compatibilizer to improve the properties of the blend to produce materials of commercial relevance. Dynamic vulcanization, a process of vulcanization of an elastomer during melt mixing with molten plastic is a typical method for producing thermoplastic elastomer vulcanizate. The improvement in toughness and impact strength of polypropylene (PP) blend with natural rubber- graft- polystyrene (NR-g-PS) is the focus of this report. Natural rubber-g-polystyrene copolymer was prepared by copolymerizing styrene with deproteinized natural rubber at 60°C using ammonium persulphate as initiator. The copolymer contained 22wt% polystyrene. Polypropylene and the NR-g-PS were mixed in an internal mixer and then dynamically curved using an efficient vulcanization (EV) system. The physio-mechanical properties of the PP/NR-g-PS blends and vulcanizates when compared with those of unmodified PP were found to be consistent with those of a toughened material: reduction in the measured values of modulus, tensile strength and hardness and increase in elongation at break and impact strength. Dynamic vulcanization was accompanied by a more than 4 - fold increase in impact strength in comparison the unmodified PP and 2 - fold increase in comparison with PP/NR vulcanizates. Scanning electron micrographs of the tensile-fractured surface showed that in contrast with the apparent brittle fractured in the unmodified PP, the fractured surface of the PP/NR-g-PS blend and vulcanizates showed moderate-to-good adhesion between the apparently well dispersed rubber phase and the PP matrix, consistent with the observed enhanced toughness of the materials.

### MP 04

**Kinetic studies on the leaching reactions in the autoclave circuit of the Tati Hydrometallurgical Demonstration Plant**  
Banyaladzi D. Paphane¹, Bonang B. M. Nkoane², Olayinka A. Oyetunji³, Ruth Gontse¹  
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Since the commissioning of the Tati Hydrometallurgical Plant (HDP), which produces Ni and Cu cathodes as well as Co salt from sulphide concentrate employing Activox Technology for leaching, no kinetic data has been generated from the plant under normal operating conditions, from start-up to steady state. Therefore, this study seeks to determine the rate of reactions of the leaching circuit with a view to obtaining kinetic data for the system under the current operating conditions. Within the 5-compartment autoclave operating at 105 to 110 °C temperature and 1100 kPa pressure, the extraction of Ni, Cu and Co into solution is achieved through the oxidation of the sulfide concentrate using approximately 50 kg H2SO4/t, 10 kg NaCl/t and 1.21 kg O2/kg S2-. Autoclave reactions showed complex kinetics, with the reactions going via some intermediate(s) before the formation of products. The results suggest that the reactions were dependent on the size of the metal ion of interest and the concentrations of the metal ions in the Tati concentrate as well as chloride leaching. The order of the leaching rate constants are Fe2+ > Cu2+ > Ni2+ > Co2+ in all the compartments studied. The rates of leaching were also found to decrease as the concentrate moves from compartment 1 to 4. For these compartments leaching was observed to be preceded by dilution of the re-pulp liquor (copper raffinate). In compartment 5, the leaching rate for this compartment was a little bit lower than that of compartment 1 but more than those of compartments 2, 3 and 4 for all the metals studied.

**MP 05 Preparation and analysis of modified clay from the local crude clay material of Nigerian origin**

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Clays have diverse use in many processing industries, agriculture, engineering practices, construction and environmental application. Clay modification however further gives better properties which the crude material does not possess. Materials of enhanced properties are most preferable especially for construction purposes where high stability and improved material properties are needed. In this work, naturally occurring clay of Ogbomosho provenience was modified with methanol and compared with the crude material for compositional changes. The basal spacing of the clay samples before and after modification was thereafter examined. Four clay samples of the same quantity was modified by ion exchange reaction using different volume of methanol in order to obtain the sample with the best outcome with respect to the extent of modification. The reaction was carried out at a temperature of 65°C for different reaction time intervals. The basal spacing of the samples which is a function of the dispersion characteristics of the methanol in the clay was determined using the XRD while the elemental composition of the samples was determined by gravimetric analysis. The XRD analysis revealed a slight increment in the basal spacing of the modified clay samples, indicating the diffusion of methanol into the silicate layers. The gravimetric analysis revealed the absence of carbon in the crude clay material, as well as a reduction in Na+ composition in the modified samples, an indication of organophilicity. The overall experimental outcome showed that the clay sample 4 (with methanol concentration of 200g/ms and reaction time of 12 minutes) gave a better outcome than the rest of the samples. It can be concluded that methanol is a viable modifier in preparation of organophillic clay of Ogbomosho provenience and that
the extent of modification is a function of several factors, out of which are the concentration of modifier and the reaction time.

**MP 06**

**Zinc Surface Modification Using Femtosecond Laser**

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Thin coatings of zinc metal grown on a glass support, using vacuum coating technology employing electron beam were treated with a femtosecond laser. The surface of the coatings was then studied for their morphology and microstructure using scanning electron microscope and x-rays diffractometers. The pristine coating was found to be crystalline in nature as shown by the Bragg peak of zinc, the evolution of the coating was shown as function of laser fluence. From the electron microscope study the morphology of the coating showed texturing which was related to the laser fluence. UV-vis-NIR response of the pristine and laser treated coating is also presented in the paper to compare it response to some transition metals that were treated with femtosecond laser.

**MP 07**

**Technical assessment of mining site and Barite quality in Nigeria**

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Barite is an exceptional non-metallic mineral composed of barium sulfate and is largely used by the oil and gas industry as drilling mud in deep drilling, where high pressure is encountered. The specific gravity of barite should range from 4.2 to 4.6 to be applicable as drilling mud. In Nigeria, barites deposits are found in veins and cavities hosted by varieties of rocks. In this work barite deposits in the various trough of Nigeria have been sampled and analyzed for the purpose of assessing their chemical composition and industrial quality. The Specific Gravity of barites in the following states Benue, Cross River, Plateau, Nassara, Jalingo and Zamfara have been analyzed using Pynometer method and their values were found to range from 3.6 to 4.3. The sedimentation process showed the particle size distribution of the barites samples to meet the specification for drilling mud. While still expecting the XRF and SEM analysis results to show the associated minerals, elemental composition and morphology of the barites samples, available results so far showed that barites samples from some locations in Cross River, Zamfara, Plateau and Nasarawa need to be upgraded through beneficiation to meet API standard required for drilling Mud.

**MP 08**

**Tailoring ball mill feed size distribution for the production of a size-graded product**

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Evidence that breakage during milling varies with material size is vastly cited in literature. This makes feed tailoring in ball milling pertinent for better grinding i.e. maximising the desired mill product at minimal costs possible. Ball mills have shown preference for finer feeds for the production of fines, however in the real world this becomes a challenge since an array of sizes is produced in each of the various stages of size reduction in milling circuits. An investigation on the best feed size distribution that could emanate in better ball milling could yield in more innovative circuit designs that could see to improved milling. To that end, batch tests were used to investigate the effect of feed tailoring in ball milling. Milling parameters of gold ore were determined using the population balance model, assuming linear breakage rate and a normalisable breakage distribution. The parameters were then used to simulate the evolution of the optimum mill product, 25-150 µm, desired for gold leaching, from different feed size distributions. The results show that feed size distribution of 0.4 0.6 0.92 1.5 5.7 7.5 15.7 70.68 mass percent of size classes 2000 1700 1170 850 600 425 300 212 µm, respectively, yields 61 % of the desired size class, when using 30 mm balls.

Production and characterization of cellulose fibre cement composites


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The increasing global thrust towards sustainability has led to the use of natural fibres or recycled fibres (obtained from various forms of waste paper) as reinforcements for the production of cement-based composites. This has led to a new approach for the industrial design of products and processes along with the implementation of sustainable manufacturing strategies to "optimize the total recycle of waste materials". Developing countries such as Nigeria possess abundant but underutilized biomaterial resources which can be harnessed for the production of sustainable building materials. This paper presents the production and characterization of fibre cement composites using recycled fibres obtained from waste newspaper and carton boxes. A slurry-dewatering process (a crude reproduction in small scale of the Hatschek Process) was used to produce fibre-reinforced cement pads with 10% by mass fraction of fibres. The composites were characterized based on physical, microstructural and mechanical (flexural strength) properties. Apparent Void Volume (AVV), Bulk Density (BD), and Water Absorption (WA) of the composites were obtained and characterized in accordance with ASTM C1185. The microstructural analysis of the Scanning Electron Microscope (SEM) images revealed a more homogenous distribution of fibres in the composites reinforced with waste newspaper fibres compared to carbon box fibres. A 3-point bending configuration was used to determine the Modulus of Rupture (MOR) for each composite. The average MOR for the saturated newspaper fibre reinforced-composites obtained was 5.80 MPa at 14 days which satisfied the minimum saturated MOR requirement (5.50 MPa) for non-asbestos fibre cement roofing products as specified in ASTM C1225-04. On the other hand, the average values for the carton box fibre reinforced composite was slightly lower (4.58 MPa). However, both composites met the ASTM C1186-02 minimum requirement of 4.00 MPa for Grade 1 fibre cement sheets. The result of this study demonstrates the potential of the use of recycled natural fibres for the
| MP 10 | **Modification of Nigerian clay for improved suitability in drilling process**  
Atitebi Zaynab¹, Falola Yusuf Ajibola¹  
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<td>The cost of the drilling fluid averages 10% of the total tangible costs of well construction. Drilling fluids are used to aid the drilling of boreholes into the earth. It is often used while drilling oil and natural gas wells. Its functions include providing hydrostatic pressure to prevent formation fluids from entering into the well bore, keeping drill bit cool &amp; clean, etc. Bentonite clays (Montmorillonite) are used in producing drilling fluid. Most bentonite clays used in Nigeria are imported from other countries; therefore, the need to modify Nigerian clay for drilling fluid arises. The clay sample used for this study was sourced from Uturu community, Isuikwuato local government, Abia state. Purification of the clay sample (Uturu 2) was done using distilled water. Also, reagents such as NaOH, KOH, NaHCO₃ and Na₂CO₃ were used to treat the clay samples at different concentrations (1.1M, 6.41M, 3.3M, 0.19M and 5.5M) and different activation time. The treated clay samples were further dried, grinded and sieved to give finer particles. The samples were then packaged and sent for analysis to determine their pH, Rheological properties and chemical composition. The result of the analysis shows that Beneficiation generally improves the pH and the Rheological properties of the clay samples compared to the untreated clay sample. Also, the XRF analysis revealed a significant exchange of higher valence cation to lower valence cation. It was concluded from this research that Uturu 2 clay sample can be suitable for drilling fluid if NaOH was used to treat it at a concentration and reaction time of 0.19M and 70min respectively. It was then recommended that additives can be added to the beneficiated clay to further improve its Rheological properties. Also, further studies can be carried out to characterize the clay sample for its mineral composition.</td>
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| MP 11 | **Preparation and analysis of modified clay from the local crude clay material of Nigerian origin**  
Adetayo Mujeeb B.¹, T. O. Salawudeen²  
¹African University of Science and Technology, (Petroleum Engineering Department, F.C.T., Abuja, Nigeria).  
²Ladoke Akintola University of Technology, (Chemical Engineering Department, Faculty of Engineering and Technology, Ogbomosho, Oyo state, Nigeria).  
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|       | Clays have diverse use in many processing industries, agriculture, engineering practices, construction and environmental application. Clay modification however further gives better properties which the crude material does not possess. Materials of enhanced properties are most preferable especially for construction purposes where high stability and improved material properties are needed. In this work, naturally occurring clay of Ogbomosho provenience was modified with methanol and compared with the crude material for compositional changes. The basal spacing of the clay samples before and after modification was thereafter examined. Four clay samples of the same quantity was modified by ion exchange reaction using different volume of methanol in order to obtain the sample with the best outcome with respect to the extent of modification. The reaction was carried out at a temperature of 650°C for different reaction time intervals. The basal spacing of the samples which is a function of the dispersion characteristics of the methanol in the clay was determined using the XRD while the elemental composition of the samples was determined by gravimetric analysis. The XRD analysis revealed a slight increment in
the basal spacing of the modified clay samples, indicating the diffusion of methanol into
the silicate layers. The gravimetric analysis revealed the absence of carbon in the crude
clay material, as well as a reduction in Na+ composition in the modified samples, an
indication of organophilicity. The overall experimental outcome showed that the clay
sample 4 (with methanol concentration of 200g/ms and reaction time of 12 minutes) gave
a better outcome than the rest of the samples. It can be concluded that methanol is a
viable modifier in preparation of organophillic clay of Ogbomosho provenience and that
the extent of modification is a function of several factors, out of which are the
concentration of modifier and the reaction time.

**Effects of Carbonitriding on case hardening of Barite mining tools**

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Barite, a chemically-stable, non-metallic mineral; with a Mohs scale hardness that ranges
between 3.0 –3.5, a density of 4.48 g/cm³ and a high specific gravity makes it a suitable
material for a wide range of applications in the oil, gas, medical, and manufacturing
industry. During mineral and mining processing of barite, relatively large amounts of
material are removed by wearing from the mining tools prior to the time when the tools
become unserviceable; with a corresponding decrease in its efficiency as a result of
changes in the dimensions of the wearing surface. The hardness of barite, together with
the impurity minerals present therein, causes both significant damage to the mining tools
and unbearable economic losses to mining investors. Failure due to wear reduces the
lifespan of the mining tool, and so increases the cost of mining of barite –in general.
Considering the socio-economic importance of barite, this work was however, aimed at
improving the wear resistance of AISI 1065 and 1070 proeutectoid steels used for (barite)
mining operations. To achieve this, the case hardening method adopted was pack-
cyaniding with dried and pulverized cassava leaves (a type of carbonitriding) at 400, 550,
800 and 950 °C for 5 h and then it was tempered at 300 °C for 3 h after that it subjected
for different kind of tests such as abrasive wear and hardness test. The implication of these
results revealed that hardening of steels with locally pulverized cassava leaves is cost
effective and environmentally safer than conventional means.

**Analysis and comparison of rheological properties of drilling mud produced from local
Baan clay and viscosifying materials (Offor) with Wyoming clay**

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Drilling of wells is an integral part of oil and gas exploration and production. The drilling
mud is the only material that remains in contact with the wellbore throughout the drilling
operations. Drilling mud cools and lubricates the drill string, it stabilizes the wellbore to
prevent rig accident. The rheology of the mud plays an important role in its performance.
The cost of drilling fluid averages 10% of total intangible costs of well construction. The oil industry is battling to cope with the dwindling oil price, a low cost and correctly formulated drilling mud can contribute to cost containment throughout the drilling process. Nigeria is blessed with a large deposit of clay. This work tends to analyze and compare the rheological properties of locally made drilling mud from local Baen clay and viscosifying material (offor) with that of imported Wyoming clay. Rheological properties of drilling mud produced from a Nigerian Local clay (i.e. Baen clay) and viscosifying material (i.e Datarium microcarpium, commonly called Offor) was investigated with Wyoming bentonite being used as a standard. It was found that properties of the mud improved appreciably when beneficiated with this local material and sodium carbonate. The excellence of the drilling mud depends on the concentration of the viscosifier. The best result which came close to the properties of Wyoming clay was Baen mud at 25g/350ml of water beneficiated with 4.0g of Datarium microcarpium (Offor). This study indicates that Baen clay has a good potential for drilling purposes when beneficiated appropriately. More experimental analysis should be done on other clay deposits, Viscosifying material (Thickeners) within and outside Niger Delta. It is recommended that experiments should be carried out to determine the effects of temperature and salt on the rheological properties of this drilling mud.

**MP 14**

**Strength and fracture toughness of laminated Bamboo panels produced from Bambusa Vulgaris**

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One of the major challenges of a developing country is unavailability of affordable housing for its ever-increasing population. This is partly due to the overdependence on high cost and non-sustainable conventional construction materials. There is therefore the need to develop an environmentally friendly and sustainable construction materials from vast natural resources available. One of these promising resources is Bamboo, an eco-friendly green material that is abundantly available. In this study, the strength and fracture properties of Laminated Panels produced from tropical Nigerian bamboo specie Bambusa Vulgaris were investigated to assess its potential for use as an alternative construction material. Round Bamboo culms were processed into strips, treated, dried and glued together in stacks to produce laminated panels which allows bamboo to be used in standardized sections and reduces its inherent variability when compared to its natural form. Tensile, Compressive and Flexural strengths of the samples were tested according to ASTM 5456 Standards for Evaluation of Structural Composite Lumber Products. The fracture toughness KIC and the resistance curve behavior of the laminates was also investigated using ASTM E399 Single End Notch bend (SENB) specimens. Results showed average values for the Tensile, Compressive and Flexural strengths (MOE & MOR) of the laminates to be of 91.57MPa, 23.51MPa, 38.18GPa and 269.9MPa respectively. The Laminated panels had comparative strength properties with some solid wood species and wood based panel boards already in use in the construction industry. The implication of the fracture behavior of the laminates are then discussed for potential applications of the laminates as an alternative construction material.

**MP 15**

**Evaluation and extraction of the Kadaure gold deposit, North-West Nigeria**

Oluwatosin Ogundipe¹, Monday Oshiogbele²
A comprehensive exploration, evaluation and extraction test of gold from the discovered ore was conducted at the vicinity of Kadaure located between longitude 6° 17′ 30″ E and 6° 20′ 45″ E and latitudes 12° 17′ 45″ N and 12° 23′ 15″ N, approximately 6 km west of Maru town, Maru Local Government Area of Zamfara State, North-western Nigeria. A detailed geological mapping on a scale of 1:20,000 was conducted across the area alongside grab sampling of quartz veins and altered wall rocks within the area. Soil samples were also collected on grid basis within the area, as part of this study. The results of the grab and soil sampling in conjunction with the geology and structures of the area were utilised in planning for an evaluation drill in the area which was used to test the continuity of the ore at depth. Furthermore, an extractive processing test was conducted across the ore body to determine the most economic and environmentally viable approach to exploit the Kadaure gold deposit. Results of exploration and evaluation shows two types of lithological units around the Kadaure area: the pelitic (mica) schist and the meta-psamite schist that have suffered from low grade regional metamorphism and a NNE-SSW foliation with steep dips to both the east and west representing tight folding around NNE-SSW axes. Both soil and grab sampling results revealed elevated values for gold in the quartz veins and altered wall rocks correlating positively with high level of arsenic and low level of lead, zinc and copper. Drilling revealed that gold occurs in quartz veins and wall rocks in the area even at depths with average and cut-off grades of 1.8g/t and 0.3g/t respectively. The processing test adopted two kinds of process flow. Process flow 1 (Gravity separation + flotation) yielding a total gold recovery of 88.85%. Process flow 2 (Gravity separation + cyanidation leaching) yielding a total gold recovery of 96.05%.

The effectiveness of application of microwave irradiation technique for enhancing the processing of low grade complex sulphide ores investigated in this research. Complex sulphide ores from two regions in Nigeria Anka (North East) and Ishiagu (South East) were selected for the investigation. Microwave treatment was performed at an intensity of 750 W for 5 minutes; and the heating response was determined after 30, 60, 90, 120, and 150 seconds. Inductively Coupled Plasma Optical Emission Spectrometer (ICP-OES), X-ray Diffractometry (XRD), X-ray fluorescence (XRF) and Scanning Electron Microscopy (SEM) were used for mineralogical characterization of the ores. Ore grindability, microhardness, froth flotation and potentiodynamic electrochemical analysis were utilized as research methods. The results show the weight percentage of lead in the ore increased with particle size reduction while weight percentage of zinc reduced with particle sizes reduction. Galena, anglesite and quartz, were identified for the as-mined Anka deposit while galena and quartz from the identified ores for the Ishiagu deposit. Microwave treatment of the ores however assisted in revealing low intensities of other phases such as sphalerite, hematite, magnetite, arsenic, and bornite in the ores. Anka deposit was observed to be richer in silica (34%) as compared to Ishiagu 4.22% silica. Hardness of the ores were

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**Effects of Microwave Irradiation technique for enhancing the processing of low grade complex sulphide ores**

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reduced after microwave treatment for various power rating, the Work Indices of Ishiagu ore by 1.32 %, 1.91%, and 1.91% after treatment for 30, 60 and 90 seconds respectively and that of Anka ore by 15.4%, 27.0% and 34.3% after 30, 60 and 90 seconds treatment respectively.

**MP 17**

**Hydration and compressive strength of Portland cement blended with kamafugites and carbonatites: Effect of physical properties**

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Two samples, a carbonatite and a kamafugite, from the Toro-Ankole geological region of East Africa are investigated for their effect on specific properties of pastes and mortars when used as natural pozzolans in Portland cement. The volcanic tuffs milled to three fineness levels, F1, F2 and F3, and blended with Portland cement at 0%, 5%, 10%, 20% and 35% replacement levels are tested for effects on hydration and compressive strength. Results show a time dependent variation in heat of hydration which increases with replacement level for the first 14 hours before decreasing. Compressive strength results show dependence on level of replacement and fineness which was pronounced until 90 days, peaking at 28 days. Increase in replacement level resulted in a general reduction in compressive strength. A conversion effect that peaks at 10% replacement level is observed in all blended samples leading to compressive strength results at 180 days being lower than those at 90 days of curing. Compressive strength test results, however, sustain the ASTM C618 and BS 3892 minimum requirement for pozzolanic Portland cements indicating that the carbonatites and kamafugites can be gainfully applied in cement production from the resource and energy economy perspectives.

**MP 18**

**Preliminary investigations on the effects of sawdust addition and partial replacement of cement with carbide waste on strength and sorption properties of sandcrete blocks**

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Housing shortage in Nigeria due to rising price of construction materials makes it logical to consider alternative building materials. Sandcrete is the main building material for walls of single-story buildings such as houses and schools in Nigeria, Ghana and many other countries in sub-Saharan Africa. As material for walls, its strength is less than that of fired clay bricks, but it is considerably cheaper. Paradoxically, many African countries are grappling with the challenges of waste management, when indeed some of the so called waste materials could be incorporated into building materials. The aim of this study was to investigate the possibility of incorporating sawdust and partial replacement of cement with welder’s carbide waste in the mix for the production of low cost sandcrete blocks. Representative samples of 100 x 100 x100 mm Sawdust-Reinforced Sandcrete Blocks (SRSB) were produced using different percentages of Teak (Tectona grandis) sawdust (20%, 25%, 30%) and welder’s carbide waste (30%, 25%, 20%) in the mix. These were cured for 28 days, after which 24-hour Water Absorption (WA), 24-hour Thickness Swelling (TS), and Compressive strength were determined. The WA (6.1 - 10.3%) and TS (1.2 - 1.9%) were quite acceptable. The mean compressive strength values ranged from 0.32 to 0.75 N/mm². The maximum compressive strength which was obtained in the SRSB mix containing 20% sawdust and partial replacement of Portland cement by up to 30% of carbide waste falls within the measured strength values (0.5 - 1 N/mm²) of commercially available sandcrete blocks in Nigeria. The preliminary cost analysis indicated the possibility
of a 20% reduction in the production of sandcrete blocks with the incorporation of sawdust and carbide waste in the production mix. It was, therefore, concluded that low cost sandcrete blocks could be produced with the addition of sawdust and partial replacement of cement with carbide waste.

MP 19

Characterization and stabilization of Laterite for sustainable construction applications
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Laterite is environmental friendly construction material that have low energy consumption, and can easily be re-cycled. The research is aimed at achieving the effective utilization of laterite as sustainable construction material by attempting to identify the best percentage of the soil stabilizers needed to improve the laterite. In this study, hydrated lime [Ca(OH)₂] and bone ash were used as a soil stabilizers to improve the strength of Nigerian laterite (gotten from Gosa and Sauka in Airport Road of the Federal Capital Territory, Abuja, Nigeria). Compressive strength, Scanning Electron Microscopy (SEM), and particle size distribution (Sieve analysis) tests were used to investigate the influence of hydrated lime and bone ash on laterite. Different percentages of hydrated lime (3%, 9% and 15%) and bone ash (5%, 10% and 15%) were used. Different methods of curing were explored to cure the cube samples. The compressive strength results showed that the addition of 9% (as the optimum amount) of hydrated lime increased the compressive strength of laterite greatly, after 28 days of curing period. In addition, the increased compressive strength of the bone ash treated samples were evident. Samples cured using air drying method of curing gave the highest compressive strength compared to the samples cured using oven drying and sun drying method of curing. From the SEM results, it was observed that the stabilization process changed the porous network of the laterite. The outcome of this research indicates positive results due to the potential of hydrated lime and bone ash to strengthen the laterite by filling the pores that exist between soil particles. It also shows that bone ash can be used in place of lime for stabilization of laterite material.

MP 20

Some problems and their remedies on development of hard and wear resistant bulk laser coating on Ti-6Al-4V
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Some remedial measures, for problems encountered during development of bulk, hard and wear resistant laser clad layers on Ti-6Al-4V was undertaken. About 50 μm thick laser clad layer having nano-structured reinforcements and a hardness of about 2250 HV could be developed by self-propagating high-temperature synthesis (SHS) of 100 μm thick preplaced powder mixture consisting of Ti, hBN, and B4C on Ti-6Al-4V substrate. On the other hand, the material could not be deposited due to powder-flying-off as a result of highly vigorous SHS in-situ reactions when a thicker preplaced powder layer (more than 300 μm) of the same composition was used. For reducing powder loss, Ni5Al and Ni
powders were sequentially used with the reactants as diluents, and material deposition was found to be improving. Furthermore, multicomponent coatings, having a thickness of 1 mm and hardness of about 1200 HV with uniformly distributed reinforcements, were developed. Ex-situ coatings were also attempted on a Ti-6Al-4V substrate using WC reinforcements. Cracks and porosities were significantly reduced in the WC reinforced coatings when Diamalloy (DA), instead of Ni, was used with WC. About 1 mm thick laser coatings with a hardness of about 1800 HV could be developed on Ti-6Al-4V using WC+DA composition. The coefficient of friction for the developed coatings was significantly low in dry sliding wear tests. Finally, grindability tests, on clad layers using WC+DA preplaced powders, were conducted to investigate the stability of clad layers, bonding strength as well as possibility of finishing the coating top surface for precision engineering applications. The hard clad layer was grindable by an electroplated diamond wheel and its strong adherence to the Ti-6Al-4V substrate was evident.

**MP 21**

**Petrological and chemical characterization of high purity quartz potential in quartzitic bodies**

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This study evaluates quartzitic bodies as potential deposits of high-purity quartz (HPQ) for use as raw materials for special applications in high-technology industries. HPQ is increasingly considered a strategic mineral in the world market due to its applications in solar, chemical, breast-tissue implants, fiber optic and other industries. In this study, we characterize quartz-vein samples in terms of their microchemical signatures and textures. Electron microprobe analysis (EMPA), particle-induced X-ray emission (PIXE) and laser-ablation inductively coupled-plasma mass spectrometry (LA-ICPMS) analyses were used to characterize the quartz varieties. These methods revealed strong Si and O signatures. Cathodoluminescence spectroscopy integrated with back-scattered electron, secondary electron images and energy-dispersive spectroscopy revealed low trace-element concentrations in some regions of the samples, and higher concentrations in some mineral inclusions. EMPA, PIXE, LA-ICPMS and cathodoluminescence studies revealed processes that led to the presence of low concentrations of trace-elements in the quartz.

**MP 22**

**High purity quartz exploration potential in SouthWestern Cameroon**

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Fluid flow along shear zones can lead to silica enrichment especially at high metamorphic grade. At various locations across the world, the silica enrichment attains a level that is exploitable as high purity quartz (HPQ). However, the details of the fluid type and mechanisms that can lead to the formation of stockwork veins of high purity quartz along shear zones are poorly understood. This study is designed to investigate recently discovered quartz-rich veins in a metamorphic terrane in Cameroon. Typically, the quartz is homogeneous and anhedral with mineral inclusions disseminated within the quartz matrix. The quartz contains medium to coarse sized grains, and varies in type from transparent to milky quartz. Euhedral mineral inclusions of mica flakes, dark radiating tourmaline and rutile needles are present in clusters within the vein. Assessment of the quartz purity was achieved Electron microprobe analysis (EMPA), particle-induced X-ray emission and Laser-ablation inductively coupled-plasma mass spectrometry (LA-ICPMS). These methods revealed strong Si and O signatures typically associated with the materials being >99.89 % SiO2. Cathodoluminescence spectroscopy (CLS) was integrated with backscattered electron imaging and energy dispersive spectroscopy to reveal complex growth textures and fracture histories of the quartz. CLS textures indicates very low trace-element concentrations that are mapped by EMPA and LA-ICPMS while higher concentrations are measured in some mineral inclusions. These mineral inclusions can be easily sorted out after mining, and before the beneficiation process. Consequently, the quality and potential quantity of HPQ veins in this area indicate a potential for HPQ exploration in the region. This discovery, together with a better knowledge of the processes leading to the formation of HPQ in quartzitic bodies, could enhance development of the mineral sector in Cameroon. This will also be useful for the exploration of HPQ in Sub-Saharan Africa, to help provide raw materials for high-tech industries such as the manufacturing of solar panels (the use of which are currently on the rise).

MP 23 Assessment of beneficiation process of a Nigerian Barite source for utilization as oil drilling mud

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The texture and size distribution of various species of gangue minerals affect the beneficiation of barite and lower the specific gravity of barite as-mined. About 97 % of the barite used in the oil industry in Nigeria is imported, even though it is found in abundance in eight states of the country. This study has examined barite from deposits in Torkula, Benue State of Nigeria for application as oil drilling mud. Physico-chemical and rheological tests were conducted, specific gravity measurements were taken along with moisture content, hardness, gel strength, plastic and dynamic viscosity. Mineral samples collected were found to have SG ranging between 3.98 and 4.42, a pH of 8.015, moisture content of about 0.161% and a Mohr’s hardness of between 3.5 and 5.0. Two sample drilling muds prepared from the pulverized barite were observed to have a mud pH of 8.65 and 11.76, plastic viscosity of 17.5 cP and 30 cP, a yield point of 24lb/ft2 and 3.5lb/ft2, gel strength
of 2.5 and 3lb/100ft² respectively. The dynamic viscosity of the drilling mud was between
0.295 and 2.755, the filtrate loss of 7.7 ml. the results were correlated with the existing
American Petroleum Institute (API) Standards. The AAS, XRD, methylene blue test and
lubricity test revealed that Nigeria barite is a potential material for oil drilling mud. Slight
beneficiation processes are required to completely refine the barite mineral from all the
associated gangue minerals, and to meet the API standards for oil drilling application.

**MP 24**

**Evaluation of Palm Oil and Palm Kernel Oil as collector reagents in Froth Flotation of Ninji Graphite**

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In froth flotation, the recovery and purity of the final product depends on various
parameters that include the type and the amount of reagent, nature and particle size of
solid, and adsorption of reagent on solid particles. Within this context, reagent type and
intended usage are important factors that are mostly considered in froth flotation. In this
work, the froth flotation performances of Ninji graphite are investigated using the
conventional collector reagent (oleic acid) and two local collector reagents (palm kernel
oil and palm oil). The froth flotation performance with the Denver flotation cell is also
investigated before conducting chemical analysis tests. The results from our study showed
that palm kernel oil is a better collector reagent compared to the palm oil, and confirmed
that the local reagents can be used in the froth flotation of Ninji Graphite.

**MP 25**

**Chaos control in the Duffing oscillator using a new method based on the damping
coefficient: numerical and electronic realization**

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This paper numerically and experimentally presents the new method to control the chaos
phenomenon in the Duffing system. Lyapunov Exponent is used as the identifier of chaos
in the system. Damping coefficient in the system is controlled to quench and also prevent
chaotic situation which are considered disturbances and also harmful for system
operations. It is found that when the depth of the double-well potential increases, the
chaos can be suppressed. The case where the amplitude and frequency of external force
are stochastic is examined. The new feedback control method based on damping
coefficient and Lyapunov exponent is proposed. The experimental investigation using
electronic components shows that the results obtained are similar to those observed from
numerical investigation.

**MP 26**

**Studies on the application of Kaolin Clay from Kisarawe District, Coast Region, Tanzania for leather processing: Part 1**

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Collagen stabilization against enzymatic attack is very crucial in biomedical industrial
applications. The present study reports the potentials of aluminium sulphate prepared
from kaolin clay as the stabilizing agent for collagen. Characterization of aluminium sulphate from kaolin has been carried out followed by crosslinking efficiency study to evaluate the interaction efficiency. FTIR and XRD results have been ascertain that kaolin would be a possible stabilizing agent for collagen to achieve heat and enzyme resistance. Crosslinking efficiency demonstrates that kaolin based aluminium sulphate is able to stabilize collagen and the stabilization efficiency increases with the increase in concentration. However, at higher concentration there is decrease in stabilization due to lowering of collagen solution pH that leads to the protonation of carboxyl group of amino acid making it unavailable to react with aluminium. From these results, it can be concluded that kaolin is the potential material for production of aluminium sulphate for collagen stabilization.

**MP 27**  
**Evaluation of the impact of solar radiation on the anti-insulation phenomenon in building energy use**  
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Before 2008, it was common knowledge around the world that insulation always saved air conditioning energy in buildings. In 2008 a phenomenon called anti-insulation was brought to light by Masoso & Grobler. They demonstrated that there are instances when insulation materials in a building directly increase building energy use. Researchers around the world then echoed the message. Recent work by some of the authors investigated the anti-insulation phenomenon in summer and winter for both hot climatic regions (Botswana) and cold climatic regions (Canada). Their study concluded that there is still a mystery of exaggerated sources of heat inside the building aggravating the anti-insulation phenomenon. They hypothesized that incident solar radiation through the windows could be one of the causes. This paper therefore focuses on eliminating direct solar radiation through windows by applying external shadings on a previously anti-insulation building. The energy saved is evaluated and the possible reversal of anti-insulation studied. The study is useful to energy policy makers and the building industry as it showcases the existence of a possible silent killer (anti-insulation) and demonstrates that investing large sums of money on insulation in buildings may not be the most economic thing to do in building design decisions.

**MP 28**  
**Replacement of conventional fine aggregates with crumb rubber in concrete – effect of particle size and volume on compressive and elastic modulus**  
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Concrete is one of the most extensively used construction material in the world. The mineral aggregates used to make the concrete are a finite resource, which is dwindling. Alternative concrete aggregates are being investigated and most recently the use of waste tyre rubber in construction has been proposed as a way of reducing the plundering of natural mineral aggregates and for curbing accumulation of waste tyres. This paper presents results of laboratory studies to investigate the effects of truck tyre crumb rubber particle size and content, as fine aggregate, on the compressive strength and elastic modulus of concrete. This is part of a broader work in progress on the characterisation of time-dependent deformation of rubberised concrete. Three tyre crumb rubber sizes (2.36 mm, 1.18 mm and 0.425 mm) were used to replace 5%, 10% and 15% by volume of fine mineral aggregates in concrete. Nine mixes were cast and tested after 3, 7 and 28 days of water curing. The elastic modulus was determined for the 10% tyre rubber – mineral
aggregate replacement concrete. The results showed a general increase in concrete workability with increase in crumb rubber content. The concrete compressive strength and elastic modulus decreases with an increase in crumb rubber content.

**MP 29**

**Kinetic Studies on the Leaching Reactions in the Autoclave Circuit of the Tati Hydrometallurgical Demonstration Plant**

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Since the commissioning of the Tati Hydrometallurgical Plant (HDP), which produces Ni and Cu cathodes as well as Co salt from sulphide concentrate employing Activox Technology for leaching, no kinetic data has been generated from the plant under normal operating conditions, from start-up to steady state. Therefore, this study seeks to determine the rate of reactions of the leaching circuit with a view to obtaining kinetic data for the system under the current operating conditions. Within the 5-compartment autoclave operating at 105 to 110 °C temperature and 1100 kPa pressure, the extraction of Ni, Cu and Co into solution is achieved through the oxidation of the sulfide concentrate using approximately 50 kg H₂SO₄/t, 10 kg NaCl/t and 1.21 kg O₂/kg S²⁻. Autoclave reactions showed complex kinetics, with the reactions going via some intermediate(s) before the formation of products. The results suggest that the reactions were dependent on the size of the metal ion of interest and the concentrations of the metal ions in the Tati concentrate as well as chloride leaching. The order of the leaching rate constants are Fe²⁺ > Cu²⁺ > Ni²⁺ > Co²⁺ in all the compartments studied. The rates of leaching were also found to decrease as the concentrate moves from compartment 1 to 4. For these compartments leaching was observed to be preceded by dilution of the re-pulp liquor (copper raffinate). In compartment 5, the leaching rate for this compartment was a little bit lower than that of compartment 1 but more than those of compartments 2, 3 and 4 for all the metals studied.
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| **CP 01** | **Environment Assisted Cracking of 316L Stainless Steel using Finite Element Approach**  
Shola K. Kolawole\(^1\), Funsho O. Kolawole\(^3\), Alfred B. O. Soboyejo\(^4\) And Winston O. Soboyejo\(^1\)  
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This paper presents the results of a combined experimental and computational study of environment assisted cracking during the exposure of 316L stainless steels to environments with different pH levels (pH of 3, 5, 8 and 11). Corrosion pits are formed on the surface of the steel, which become likely initiation sites for stress corrosion cracking. The transition from pits to cracks is elucidated via confocal microscopy and scanning electron microscopy. The stress concentrations associated with possible pit sizes and configurations are also modeled using finite element analyses and fracture mechanics models. The resulting cracks can also grow by stress corrosion cracking mechanisms, when the applied remote stresses exceed the threshold crack driving force. |
| **CP 02** | **Density Functional Theory Study of Oxygen Co-Adsorption on Li/Na Adsorbed Mo\(_2\)(110) Surfaces (M=Mn, Ti And V)**  
Khomotso Maenetja\(^1\), Ricardo Grau-Crespo\(^2\) and Phuti Ngoepe\(^1\)  
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Lithium air batteries have been studied extensively whereas operation of sodium-air batteries has just gained attention recently. Catalytic effect on the performance of sodium air battery has not been an area of interest yet. However, it has been reported that the most stable product in Na-air battery is NaO\(_2\) whereas in Li-air battery it has been reported that the major and stable product is LiO\(_2\). In this work, we present density functional theory study of how metal oxide (MnO\(_2\), TiO\(_2\) and VO\(_2\)) catalyst affects nucleation of LiO\(_2\) and NaO\(_2\) and other products that may be formed. We further investigate the discharge products of these two metal air batteries compared to the known systems of the product in terms of their formation energy and their morphology. Look into the O-O bond length which plays an important role in Oxygen Reduction Reaction (ORR) during discharge of the battery. Interestingly it has been found that what was reported in literature, that the most stable products in Na-air batteries being NaO\(_2\) is indeed what has been observed in our study. Furthermore, the type of structure that has been found was the pyrite form whereas the most stable product in Li-air battery, LiO\(_2\) has the hexagonal type. Amongst the three metal oxides it can be concluded that MnO\(_2\), is the most favourable catalyst because it encourages the formation of the reported stable products in both metal air batteries. |
| **CP 03** | **Reliability and Performance Modelling of Solar Powered Street Lighting Systems**  
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This paper presents the combined results of analytical and computational modelling of the reliability and performance of the solar-powered street lighting systems installed at the African University of Science and Technology (AUST) in Nigeria, a hot and humid environment. The technical performance of the systems was studied using the following performance indicators: system energy yield, capture loss, as well as the system performance ratio while the reliability of the systems was examined using a model developed from the findings from the maintenance and fault diagnosis of the systems. The model was used to predict the total failure and survival probability of the systems using the Weibull distribution. The performance evaluation during the monitored period (February 2012 to January 2015) indicated that the performance ratios of the systems vary from 70% to 89% and the energy yields of the systems ranging from 2.87 h/day to 5.57 h/day. The results from the reliability analysis also showed that when the stress concentration factor around the notch between the cable terminals in the charge controller increases, the charge controller will become overheated, which in turn affected other components of the systems. The implications of this study are also discussed for the design and development of future solar-powered street lighting systems.

**CP 04**

**Analysis of Nonlinear Heat Transfer in a Cylindrical Solid with Two-Step Exothermic Kinetics and Radiative Heat Loss**

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This paper examines the problem of nonlinear heat transfer in a cylindrical solid of combustible materials with two-step exothermic kinetics and radiative heat loss to the ambient surrounding. The reactant diffusion and temperature-dependent pre-exponential factors with respect to sensitized, Arrhenius, and bimolecular kinetics are taken into account in the model energy balanced equation. Both regular perturbation method and numerical shooting technique coupled with Runge-Kutta-Fehlberg iteration scheme are employed to tackle the nonlinear model problem. The effects of various thermophysical parameters on the reactive cylindrical solid temperature, Nusselt number and thermal stability are discussed quantitatively with the help of computational illustrations. It is found that radiative heat loss enhances thermal stability of the material while the two-step exothermic kinetics promotes the onset of thermal instability.

**CP 05**

**Applied Mathematics And Numerical Computation To The Benefit Of Modern Material Sciences**

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In this report, we give a general review of the possible areas, in which the methods of applied mathematics may be implemented to the benefit of modern material sciences. In particular, we address the emerging framework of nano-technologies, and discuss both the issue of modeling, as well as that of solving (typically, by approximate/numerical methods) the mathematical problem as presented by the model. We also emphasize the crucial role of close collaboration between the mathematicians on one side, and scientists and engineers on the other side, for the overall success.

**CP 06**

**Adaptation of a Hybrid Automatic Process Control System for the Operationalisation of Mineral Processing Plants, using the Barite Beneficiation Plant as a Case Study**

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Over the years, the focus of recent technological revolutions in the design of barite processing plants has dwelt on the manufacture of state-of-the-art beneficiation machinery which were merely aimed at processing barite ores from specific sites. Although the support for the current design methodology for barite processing/beneficiation plants could be justified by the fact that different barite mining sites pose different design challenges to barite processing engineers, it is common knowledge that the current design methodology places heavy economic and man-power burdens on barite processing industries. In order to address this problem, this work considered the possibility of retrofitting the existing plant designs for barite processing with a hybrid automatic control system which would revolutionalise the process throughput, regardless of the geographical peculiarities of the mining site and the variations in the site-imposed properties of barite ores. The automatic control system was designed by superimposing a feedforward control system on a feedback control system. The design of the automatic control system was analysed by the method of direct substitution. The governing equations used in analysing the barite beneficiation process, as well as the applicable equations which modelled the disturbance in the beneficiation process were derived from first principles – using transfer functions and block diagram representations. The performance of the automatic control system was simulated with the aid of computer software; and the results obtained from the simulation showed that the response of the automatic control system for the barite beneficiation process was stable, but oscillatory.

Cluster ions have attracted the interests of many researchers due to their unique electronic, optical and magnetic properties. They are applicable in ion thrusters, ion implantation technologies, magneto hydrodynamic generators and aerospace investigations amongst others. Positive ions Ba2X3+, Ba3X5+ and Ba4X7+ (X=F, Cl, Br or I) and negative ion BaCl3– have been detected earlier experimentally. However, there are no experimental data about the geometrical structure, vibration spectra and thermodynamic properties of these ions. In this work, the geometrical structure, vibration spectra and thermodynamic properties of these ions were obtained using computational methods. The calculations were performed using the Firefly software. The electron density functional theory with the functional B3P86 and the second and fourth order Møller–Plesset perturbation theory were used. For the barium atom, the ECP with def2-TZVP basis set has been applied while for the halogens, the Dunning, McLean-Chandler, aug-cc-pVTZ, SDB-aug-cc-pvtz basis sets were used accordingly. The theoretical and based on experiment values of ΔfHo(0) were computed. The equilibrium structures of the ions BaX3–, Ba2X3+, Ba3X5+ and Ba5X9+ correspond to D3h and Ba4X7+ to C2v symmetry. The values of ΔfHo(0) of the species were determined (in kJ mol−1): −1356 ± 4 (BaF3–); −1039 ± 12 (Ba2F3+); −2179 ± 16 (Ba3F5+); −3277 ± 35 (Ba4F7+); −4316 ± 22 (Ba5F9+); −1859 ± 7 (Ba2F4); −858 ± 6 (BaBr3–); −293 ± 10 (Ba2Br3+); −982 ± 20 (Ba3Br5+); −1644 ± 30 (Ba4Br7+); −2282 ± 17 (Ba5Br9+); −709 ± 6, (BaI3–), −96 ± 12 (Ba2I3+), −654 ± 17 (Ba3I5+), −1177 ± 20 (Ba4I7+), and −1686 ± 20 (Ba5I9+). The theoretical results of ΔfHo(0) for the ions studied agree well with the results based on experiment. Therefore, these results compliment experimental results and confirm the existence of the ions above.
CP 08  
First Principle Study of the structural and electronic properties of GaSb and InSb semiconductors in zinc blende, rock salt and wurtzite phase
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We have performed first principle calculation to determine the structural and electronic properties of GaSb and InSb semiconductors in three different phases; Zincblende (ZB), Rocksalt (RS) and Wurtzite (WZ). The structural properties which includes the equilibrium lattice parameter, Bulk modulus and phase transitions is obtained by performing a structural optimization method using the GGA-PBE as the exchange correlation. Our calculations showed that both GaSb and InSb are more stable in the ZB phases. We also observed that under pressure, a phase transition from ZB to RS occur at 8.03GPa for GaSb and 9.72GPa for InSb. The energy band structure for the three different Phases was also investigated in details. A transition from the semiconducting ZB phase to metallic RS Phase is observed for both GaSb and InSb. Our result show an overall agreement with experimental results.

CP 09  
Ab Initio Investigation of Electronic, Structural and Lattice-Thermal Properties of Zincblende Indium Nitride (InN)
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The group-III nitrides semiconductors are currently investigated due to their promising application in short-wavelength electroluminescence and high-power electronic devices. A very important member of the group-III nitrides is Indium nitride. Here we report first-principles density functional theory calculation of the electronic and structural properties of Indium nitride (InN) in zincblende structure. The calculated ground-state properties such as the lattice constant, bulk modulus and its pressure derivative as well as the optical band gap energy are in reasonable agreement with available theoretical and experimental data. We also determined the temperature dependence of the lattice thermal conductivity of InN between 0K and 1500K using Density Functional Perturbation Theory (DFTB) and Linearized Boltzmann Transport Equation (BTE) within the Single time Mode Approximation.

CP 10  
Effect of Polymer Tacticity on the Structure and Glass Transition Temperature of Supported Polystyrene Thin Films
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We have used all-atom molecular dynamics (MD) simulations to investigate the effect of tacticity on the structure and glass transition temperature (T_g) of polystyrene (PS) thin films adsorbed on two distinct types of solid substrates. The systems consist of thin films made of atactic, isotactic, and syndiotactic PS films supported by graphite or a-quartz substrates, which are known to be atomically flat but chemically and structurally different. We have observed a marked dependence of the film structure on substrate type as well as on tacticity. For instance, rings orientation near substrate surfaces depends on substrate type for aPS and iPS films while no such dependence is observed for sPS films whose interfacial structure seems to result from their propensity to adopt the trans conformation rather than their specific interaction with the substrates. Moreover, our
results indicate that glass transition temperatures of substrate supported polystyrene films are higher than those of the corresponding free-standing films. More specifically, PS films on graphite exhibit large $T_g$ values compared to those on $\alpha$-quartz, and we have noticed that syndiotactic PS has the largest $T_g$ irrespective of substrate type. Substrate-film interaction energy and chains’ dynamics near substrate-film interfaces were subsequently investigated in order to substantiate the obtained $T_g$’s and, it was found that films with higher $T_g$’s are strongly adsorbed on the substrates and/or exhibit a smaller interfacial chains dynamics due essentially to steric hindrance.

CP 11  
**Design of High Efficiency Tandem Solar Photovoltaics: Mathematical and Computational Approach**  
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Solar photovoltaics represent one of the world’s most promising sources of renewable energy generation. In fact, calculations based on thermodynamics demonstrate that the limit on the conversion efficiency of sunlight to electricity is about ninety three percent. Sadly, first generation solar photovoltaics, largely available monocrystalline and polycrystalline bulk silicon, exhibit about seventeen percent actual efficiency, while second generation solar photovoltaics, largely thin films, exhibit actual efficiency even far less. This is due to their single band gap which guarantees that they can never exceed the theoretical efficiency limit of about thirty-three percent known as the Shockley-Queisser limit. In 1955, Jackson suggested that this limit can be circumvented through multiple energy thresholds by stacking of P-N junctions in different semiconductor materials, thus giving rise to third generation solar photovoltaics, mainly tandem photovoltaics. To minimize experimental cost, it is important to know what efficiency is to be expected for a given choice of material system (bandgap, thickness, junction depth and doping characteristics during epitaxial growth) and configuration (stacking/layering and contacts/connection) using appropriate mathematical formulation (model) and computation. Hence, we recognize this as a variational inequality and fixed point problem. Consequently, we construct and study a gradient method iterative process for approximating a common element in the set of fixed points of relatively non-expansive maps and the set of solutions of variational inequality problems for monotone, k-Lipschitz maps in 2-uniformly smooth and 2-uniformly convex real Banach spaces. We prove a strong convergence theorem for a sequence generated by this process to that common element. We then define some associated physical quantity functionals and perform numerical experiments and simulations using the iterative scheme. We obtain interesting and significant results.

CP 12  
**Analysis of Blasius Flow of Hybrid Nanofluids Over a Convectively Heated Surface**  
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This article explores the problem of Blasius flow of water based hybrid nanofluid containing $\text{Al}_2\text{O}_3$ and $\text{Cu}$ as nanoparticles over a convectively heated surface. Five different geometries of nanoparticles shape viz spherical, bricks, cylindrical, platelets and blades are considered in our analysis. The nonlinear model equations are obtained and tackled numerically using shooting method coupled with Runge-Kutta Fehlberg numerical scheme. The effects of nanoparticle shapes and other relevant thermophysical parameters on fluid velocity, temperature, skin friction and Nusselt number are discussed with the help of computational illustrations. The result for skin friction coefficient is compared with already existing results in the literature and excellent
agreement was obtained. It is found that the heat transfer rate of hybrid nanofluid (Cu-Al₂O₃/Water) is higher than that of nanofluid (Al₂O₃/Water) and the Nusselt number increment for blade shaped nanoparticles is the highest as compared to that of platelet, cylindrical, brick and spherical shaped nanoparticles.

**CP 13**

**Photovoltaic properties of CuxAlyS₂ thin films deposited by chemical-bath deposition**  
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**CP 14**

**Early detection and diagnosis of triple negative breast cancer in contrast-enhanced resonance image using Texture Features and support vector Machine**  
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Triple negative breast cancer is most common and leading cause of cancer death among African women. It has become a major health challenge in the black race over 5 decades, and its occurrence has risen in recent years. Early detection is an effective way to diagnose triple negative breast cancer. Computer-aided detection or diagnosis (CAD) systems can play a vital role in the early detection of triple negative breast cancer and can reduce the death rate among black women with triple negative breast cancer. Support Vector Machine (SVM) is used for classification. The Support Vector Machine (SVM) is implemented using the kernel Adatron algorithm. The kernel Adatron maps inputs to a high-dimensional feature space, and then optimally separates data into their respective classes by isolating those inputs, which fall close to the data boundaries. To enhance the contrast of the input image, identify the region of interest and detect the boundary of the breast pattern, DCE-MRI breast cancer imaging has been chosen, and the triple negative breast cancer tissue with magnetic nanoparticle. The proposed neural network model hold promises for radiologists, surgeons, and patients with information, which was previously available only through biopsy, thus substantially reducing the number of unnecessary surgical procedures. For training and testing the neural network, we used dataset made available to us by our collaborators at Worcester Polytechnic Institute (WPI) Massachusetts, USA. To evaluate its performance, the C-means (CM) classification method is compared with SVM. By some experiments, the result of SVM is better than C-mean.

**CP 15**

**Computational modelling of B19 Ti-Pt-Zr in High Temperature Shape Memory Alloys applications**  
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High temperature shape memory alloys are being developed in order to increase the application area of shape memory alloys. There is an increasing demand of shape memory alloys which can be used at high temperatures in the aerospace, energy, actuators and sensors in automotive. This unique behaviour is due to shape memory effect and superelasticity as a results of phase transformation. The semi-empirical embedded atomic method interatomic potentials incorporated in the LAMMPS code employed to investigate the mechanical and temperature dependence of the Ti50-xZrxPt50 ternaries at various temperature ranges. The lattice parameter increase with Zr addition, the heats of formation is more stable at 5 at.% Zr, The elastic properties for 5 at.% Zr showed positive shear modulus indicating the stability of the structures at 0K. The martensitic transformation of Ti50-xZrxPt50 (x= 5) was observed around 1200K where the lattice ratio a\b or
c\b was 1.55 which confirmed B19 to B2 transformation. The transformation temperature of the ternary structure is lowered from 1285K TiPt to 1200K with the addition of 5 at.% Zr.

**CP 16**

**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/SeS\textsubscript{x} 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/SeS\textsubscript{x} 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 Li\textsubscript{2}S and Li\textsubscript{2}Se, which agreed with available experimental results. A cluster expansion technique 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 Li\textsubscript{2}S and Li\textsubscript{2}Se were derived and validated and used to explore high temperature structural and transport properties of mixed systems.

**CP 17**

**DFT study of bulk cadmium oxide: The effect of exchange-correlation functionals on the equation of states**  
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Cadmium oxide is a transition metal oxide with interesting properties and wide industrial applications. The states and thermodynamic properties of such materials are well described by the equation of state. This work employed the *ab initio* methods to study the equation of states of cubic cadmium oxide. All calculations were done within the density functional theory framework and the plane wave basis set as implemented in the QUANTUM ESPRESSO computer code. The effect of various exchange-correlation functionals on the equations of states was deeply investigated and a comparison with previous theoretical and experimental works presented.

**CP 18**

**First-principles Study of Mn-doped Defective Graphane Monolayer**  
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Recently, it has been established that the electronic properties of hydrogenated graphene (graphane) sheet can be well tuned by foreign atom substitutions. This suggests that incorporating magnetic elements into its semiconducting environment could make graphane a good base for creating low dimensional dilute magnetic semiconductors for spintronic devices desirable for information storage and processing. Using density functional theory including the GGA + Hubbard U correction, we investigate the effects on structural, electronic and magnetic properties of graphane upon incorporation of Mn adatom on different adsorption sites. It is found that the high-
Spin configurations are more favourable for all the considered defect systems regardless of the adsorption sites. The Mn adatom shows appreciable preference to substitute the H vacancy site yielding a supercell magnetic moment of 6.0 μB, while subsequent adsorption of H on top of Mn enhances stability of the defect. The rich magnetic properties of these systems are particularly important for efficient spin injection and transport of high spin polarized currents, desirable in spintronic device applications.

**CP 19**

**Computational Principles On Feal-X (X=Pt, Ru)**  
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The Fe-Al based systems have recently attracted a lot of attention as potential alloys in many applications due to their excellent resistance to oxidation at high temperatures. Fe-Al are treated as “the materials of the future”, for constructional and coating, for high temperatures applications in aggressive and corrosive environment. However, they suffer limited room temperature ductility and a sharp drop in strength above 600 °C. The current study employed density functional theory approach to investigate the stability of FeAl-X alloys. Density of states were used to describe the behaviour of each phase near the Fermi level; these phases were observed at different percentage compositions. We employed virtual crystal approximation (VCA) to model various atomic concentrations (0 ≤ x ≤10) for both Pt and Ru. Addition of Pt and Ru was found to significantly improve the ductility of the FeAl-X compound for 0.2 and 0.5 at. % composition, respectively.

**Keywords:** FeAl-X alloys, DFT, Heats of formation, Density of states, X-ray diffraction patterns.

**CP 20**

**Computational modelling studies of martensitic transformation of TiPd shape memory alloys.**  
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We use density functional theory to investigate the martensitic transformation of TiPd shape memory alloy employing pseudopotential plane wave methods within the Pardew-Burke-Ernzerhof Generalized Gradient Approximation (PBE-GGA).The electronic, phonon dispersion, and elastic constant were determined to check the stability of TiPd alloy for B2, L10, B19 and B19’. The lattice parameters and heats of formation are well in agreement within 3% with the available experimental data for B2, L10, B19 and B19’ in TiPd. We found that the calculated heats of formation and density of states predicted B19’ TiPd to be the most stable structures compared to B19, B2 and L10. The B2 TiPd phase is found to be mechanically unstable with respect to the monoclinic B19’ structure in agreement with phonon dispersion curves. The temperature dependence of the B19 and L10 TiPd structures were investigated using embedded atom method in the LAMMPS code. The a and c lattice parameters increase with an increase in temperature in B19 and L10. In L10, a and b lattice parameters there are extreme increase observed while in c lattice parameter and c/b ratio there are extreme decrease observed at temperature 897.1K which suggest that L10 phase has transformed to B2 phase. The ratio c/b of the B19 TiPd is 1.414 at approximately 1496.4K which suggest that B19 phase has transformed to the cubic B2 phase. The elastic constants and shear modulus of B19 and L10 decreases with an increase in temperature.

**CP 21**

**The effect of Co and Sn on Zr-Nb alloys for high temperature application**  
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Zirconium has attracted a lot of attention recently due to its distinctive properties that make it suitable for extensive applications in the nuclear power and chemical industry. Zirconium and its
Alloys are undergoing long-term development as promising materials for the nuclear industry and power engineering. Recently, advanced Zr-based alloys are aimed for service in more severe operating conditions such as higher burn-up, increased operation temperature, and high-pH operation. In this work we observe the temperature dependence of Zr50Nb50, Zr78Nb22, Zr78Nb19Co3 and Zr50Nb49Sn1. It was observed that ternary additions with small atomic percentages of Co and Sn have significant impact on ZrNb alloy; and their elastic properties showed a possible enhancement on high temperature applications and physical strength.

### CP 22

**Theoretical computer modelling studies of electronic and mechanical properties of kaolinite clay mineral.**

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Kaolinite [Al₂Si₂O₅(OH)₄] is one of the most desired and common clay mineral under the serpentine group, which also includes dickie, nitrile and halloysite polymorphs. This mineral is best known for its good structural, physical and mechanical properties such as whiteness, non-abrasiveness, low ability to absorb water and exchange ions. These properties make Kaolinite to be an ideal applicable mineral for ceramics, paint, papemaking, tyres, rubber, cables, ink and pharmaceutical purposes. Furthermore, these properties increase the strength and durability of the mineral, and also enhance the good appearance of kaolinite products. Kaolinite can either be found dominant in clay mineral or as an entire deposit of clay. However, little has been reported on the structural, electronic and mechanical properties of Kaolinite which are essential for its application. In this work, computational modelling techniques have been employed to the study the structural, electronic and mechanical properties of Kaolinite, particularly, cell parameters, band structure, density of states (DOS) and elastic constants. All calculations were performed using the density functional theory (DFT), using CASTEP code within material studio interface. The calculated cell parameters are in good agreement to the experimental data to within less than 1%. The band structure calculations showed that Kaolinite has a band gap of 5.062 eV, suggesting insulator behaviour. Furthermore, the plotted DOS also suggest insulator behaviour. Finally the calculated elastic properties are independent and impose no restrictions to each other.

### CP 23

**Determination of the Relaxation Time Constant for Electron Scattering in Gallium Arsenide (GaAs) and in Methylammonium Lead Iodide Perovskite (CH₃NH₃PbI₃)**

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One of the biggest obstacles to technological development in Africa is insufficient supply of electricity to most parts of Africa while other developed countries of the world also depend on fossil fuels which contribute to environmental pollution. An attractive alternative source of energy which solves the problem of insufficiency and is a clean source of energy is solar energy. In order to extract energy from the sun, photovoltaic cells with semiconductors as light absorbers can be used to convert the light energy from the sun into direct current. Gallium Arsenide (GaAs) and Methylammonium Lead Iodide (CH₃NH₃PbI₃) perovskite are solar cell material absorbers with efficiencies that surpass that of Silicon. Scattering of charge carriers in these materials reduces the corresponding relaxation times of carriers and thus, decreases the efficiencies of the solar cells. Contributions to the relaxation time come from scattering by impurities or different modes of phonons. These scattering mechanisms limit the mobility of carriers. In this study, we analyze the scattering mechanisms that limit carrier mobility in GaAs and CH₃NH₃PbI₃ perovskite.
Subsequently, the carrier effective masses and relaxation times were evaluated. The relaxation times are calculated using the Fermi golden rule while the effective masses are derived from the respective electronic band structures. The carrier mobilities are then evaluated using deformation potential theory. The effect of strain on the relaxation time is also reported. The required band structures and energies were calculated using the Quantum ESPRESSO code under the framework of density functional theory (DFT).

**CP 24**  
**Structural and Electronic Properties of van der Waals Heterostructures**  
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Two-dimensional (2D) materials and their heterostructures are useful in electronic applications, especially with the drive towards more and more miniaturization. Using ab initio methods, we study the structural and electronic properties of van der Waals heterostructures of 2D materials namely hexagonal boron nitride (hBN), black phosphorous and some transition metal dichalcogenides and diselenides (MoS\(_2\), MoSe\(_2\), WS\(_2\), WSe\(_2\)). Our studies were based on density functional theory (DFT) as implemented in the Quantum ESPRESSO program. 2D layered materials present a huge challenge for DFT as a result of interlayer van der Waals (vdW) interaction which is absent from the typical DFT exchange-correlation functional. In order to account for the van der Waals interactions between layers, we applied the semi-empirical DFT-D2 method of Grimme and the revised Vydrov–Van Voorhis non-local correlation functional (rVV10). We show that the two approaches give similar structural properties of the van der Waals heterostructures. We also found that via the application of a perpendicular electric field, it is possible to tune the size of the electronic band gap of these structures.

**CP 25**  
**Performance Analysis and Optimization of Iterative Kohn-Sham Solvers with Application to Semiconductor Quantum Dots**  
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Kohn-Sham (KS) density functional theory (DFT) is a computational quantum mechanical modeling method used to investigate the electronic structure of many-electron systems (atoms, molecules, and solids). The method leads to the so-called Kohn-Sham equations which lead to be solved (diagonized) iteratively, on approach call self-consistent-field (SCF) iteration. These SCF iterations can require huge computation resources and thus, depending on the size of the physical system under consideration. A number of solvers with difference efficiency efficiencies have been developed for this task. A performance analysis of four different Kohn-Sham solvers [Conjugate Gradient (CG), Davidson, Projected Precondition Conjugate Gradient (PPCG) and Parallel Orbit Update method (ParO)] was carried out. The solvers were parallelized in the band-group using message-passing-interface (MPI) libraries. The times for diagonalization of the KS equations for system with 4096 atoms of Silicon (Si), Cadmium Telluride (CdTe) and Zinc Sulphide (ZnS) with increasing number of processors were recorded. With the Parallelization in the band-group the Conjugate Gradient method turned out to perform best. As an application of the finding of this work, CdTe and CdSe Quantum dots were studied, which have applications to solar cells, and their electronic densities of state (DOS) and absorption spectra will be presented.

**CP 26**  
**Investigation of Lithium-ion Solvation and Diffusion in Ethylene Carbonate Using Classical Molecular Dynamics**  
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Lithium-ion (Li+) battery performance is highly dependent on the choice of the materials for the electrolyte solution. Currently a common choice for rechargeable Li-ion batteries is a lithium salt dissolved in an organic solvent. Understanding the solvation of the salt in the solvent is, therefore, crucial to understanding the ion transport across the battery during charge and discharge. In this work we study the behavior of lithium hexafluorophosphate (LiPF6) in ethylene carbonate (C3H4O3) using classical molecular dynamics and model potentials implemented in the Large Scale Atomic/Molecular Massively Parallel simulator (LAMMPS). We analyze the solvation structures of both Li and PF6 ionic groups in C3H4O3 and compare the results with existing DFT calculations in order to determine whether the ReaxFF classical model potential used to model the interatomic behaviour can reproduce the critical aspects of the solvation. Finally we calculate the diffusion coefficient of Li+ in the electrolyte from the slope of the Mean Square displacement (MSD) and compare with experimental findings.

There is a search for excellent cathode materials for lithium ion batteries (LIB) in order to meet the requirements of low cost, high safety, and high energy capacity in many applications of the battery. Manganese dioxide (MnO2) is a semiconductor material and it is a promising electrode material due to its ease of preparation, low cost and low toxicity. It has been widely used for commercial primary lithium batteries and has attracted attention because of its high stability and high capacity for lithium adsorption. MnO2 can be found in different phases, such as α-MnO2, γ-MnO2, λ-MnO2, and β-MnO2 can accommodate significant lithium in their cavities, showing large capacities as cathode materials for LIBs. In this work, the lithiation process of these phases has been systematically examined by first-principles calculations within the local density approximation (LDA) or generalized gradient approximation (GGA) of the density functional theory (DFT), the relative stability before and after the lithium intercalation process were firstly determined. The electronic properties, electrochemical potential and volume change upon insertion of Lithium for each of the phases were also determined. Our results indicate that α-MnO2 and β-MnO2 manganese oxide are best suited as cathode materials for high capacity Li-ion batteries.

Liquid crystalline dendrimers (LCDrs) are part of dendrimers which usually are derived through functionalization of common dendrimers with low molar mass liquid crystal molecules. Inclusion of anisotropic molecules into nearly spherical dendritic scaffolds enables to obtain multifunctional
anisotropic macromolecules. This opens up the possibility of achieving a wide variety of physical properties with tailor-made potential applications. Controlling microscopic or macroscopic alignment of liquid crystalline dendrimers (LCDrs) in an external aligning field is an important feature for their possible potential applications. In this presentation, we mainly focus on the investigation of structural and alignment properties of (a) single LCDrs of different generation and functionality confined in a single flat wall (b) system of LCDrs of a given generation and functionality confined in a slit pore of two parallel impenetrable walls whose inner surfaces induce several types of anchoring styles and (c) single LCDrs of different generation under smectic like mean fields. Monte Carlo computational simulation method has been used to study those properties of mentioned systems. In each system the size, shape, distribution and alignment properties of LCDrs have been well studied. In the case of confined LCDrs in a single wall and slit pore, distribution of dendritic segments and ordering of mesogenic units along the direction perpendicular to the confining surface were addressed. More importantly, the propagation of ordering (position and orientational) from the vicinity of the confining surface to the bulk region was the key information we had to investigate. When it comes to LCDrs under smectic like mean fields, LCDrs are exposed to an external electric/magnetic like mean field which acts only on the orientation of mesogenic units therein disturbing the overall shape and size of the whole molecule. In this case, varying field strength and some other parameters, we have studied sub-partitioning of dendritic segments, stretching and compressing of thewhole macromolecule. The LDr studied here represents a wider range of polyphilic mesomorphic materials in which separate building blocks with different types of interaction sites are combined. External mean field induced micro-phase separation and alignment transmission in these materials opens up the opportunity to self-assemble in to well-defined nanostructures for different potential applications. The CG-simulation method presented here can be used as an inspiration towards further simulation and experimental studies on these systems. As a result, it could be a useful tool in helping design confined nanoscale structures for future applications.

CP 29 Molecular dynamics simulation of the interfacial thermal resistance between phosphorene and germanium substrate
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The concept of heat management is a major factor militating against the optimum performance of microelectronic devices most especially in Africa where the effect of hot weather can be a contributing factor. As the maximum power rating of a transistor is limited by the temperature of the junctions, it is necessary to make the right material selection for the thermal interfaces such that the heat generated can be dissipated as quick as possible and avoid over heating of devices. Phosphorene, a recently discovered two-dimensional material, is poised to show some distinguishing characteristics in both thermal and electrical properties. It has exhibited the quality of being a good thermal interface material. In this work, we study the dynamical response of phosphorene to thermal impulse using the transient pump-probe technique and evaluated the interfacial thermal resistance (R) between Phosphorene and a Germanium substrate. We also investigated the effect of substrate thickness on R. A germanium substrate was investigated because of its potential use in next-generation high-frequency transistors. The studies were carried out using molecular dynamics simulations.

CP 30 The Effect of Temperature in Li_{0.07}TiO_2 Nanoporous for Electric Energy Storage in LIBs Applications. The Effect of Temperature in Li_{0.07}TiO_2 Nanoporous for Electric Energy Storage in LIBs Applications. The Effect of Temperature in Li_{0.07}TiO_2 Nanoporous for Electric Energy Storage in LIBs Applications.
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Various polymorphs of titanium dioxide (TiO$_2$) are widely used as anode materials in Li/TiO$_2$ batteries. Electrolytic TiO$_2$ is the most electrochemically active form of TiO$_2$ and is very difficult to characterize. Their structural details are still largely unknown owing to the poor quality of X-ray diffraction (XRD) patterns obtained from most TiO$_2$ samples. Nanoporous Li$_{0.07}$TiO$_2$ architecture structure was recrystallized, cooled and heated using molecular dynamics simulation technique. Recrystallisation was confirmed by RDFs and the change in configuration energy with time. Li diffusion increases with an increase in temperatures. The temperature variation shows to have no effect on the Li$_{0.07}$TiO$_2$ nanoporous structure, where both sliced microstructures and XRDs patterns display the presence of rutile and brookite polymorph.

**CP 31**

**Electronic Properties of Layered Semiconductor materials**

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Accurate electronic band structure calculations are the first step in any electronic properties calculations concerning semiconductor materials. The empirical pseudopotential method extended to the large basis approximation was used to determine the electronic band structures of layered semiconductor materials. In order to achieve accuracy in the band structure calculations, optimized continuous atomic form factor potentials obtained through the Levenberg-Marquardt algorithm and cubic spline interpolations are used. Our results are compared with those obtained through standard Density Functional Theory calculations and experiments.