SAIP2023

Monday 03 July 2023 - Friday 07 July 2023

University of Zululand

Book of Abstracts

Contents

Poster Session 1 / 2

Graphene/TiO2 as electron transport layer to enhance energy efficiency of perovskite solar cells

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In the field of the energy transition, developing efficient and cost-effective solar cells is a crucial goal to establish an optimal energy mix. The third generation of photovoltaic cells, which utilize abundant materials and simple processes, has emerged to achieve this goal. Among these, photovoltaic cells based on perovskite materials have demonstrated significant advances, with power conversion efficiencies reaching up to 22%. However, efforts are still needed to improve these cells' charge generation and collection. One strategy to achieve this is using TiO2/graphene nanocomposites, which have been shown to reduce recombination phenomena and improve electron collection. The technique of laser pyrolysis is used to achieve high-quality nanocomposites with suitable properties for efficient and stable solar cells. This technique enables the synthesis of nanoparticles in a single step with a continuous flow. Tests were conducted using a MAPI-Cl perovskite deposited in a single-step, and the results show an increase in electron injection efficiency and device performance with the use of graphene in the mesoporous TiO2 layer. Overall, the use of this technique resulted in an increase in power conversion efficiency from 14.1% to 15.1% for these devices, demonstrating the benefit of the laser pyrolysis process for the production of high-quality electron transport layers in perovskite solar cells.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / 4

A mechanistic non-process dependent study of the prediction and optimization of mineral beneficiation and metal extraction.

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Abstract. Process prediction and optimisation have been regularly conducted in physical systems. While most of the tools used require the introduction and analysis of input–output parameters, often ranges of values are required. The observed non-personalisation of the range of input parameters and the obtained outcome values in the metallurgical processes has prompted the content of this paper. For the same range of values introduced into the input layer of an artificial neural network frame, with the very same weight and boundary conditions would lead exactly to the same outcomes

interpretation of which is process dependent. The paper will discuss the case of concentration of sulphide minerals through flotation compared to the case of the dissolution of cobalt-bearing minerals in an acid solution before ending with the calcination and roasting of a sulphide. A demonstration of the non-specification of the outcome of the physical systems will be discussed.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MEng.

Consent on use of personal information: Abstract Submission:

Nuclear, Particle and Radiation Physics / 5

Axion-Like Particles at Future $e^{-}p$ Colliders

Authors: Karabo Mosala[1]; Mukesh Kumar[1]; Goyal Ashok[2]; Pramod Sharma[3]

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In Beyond Standard Model (BSM) theories, Axion-Like Particles (ALPs) are hypothesized to be Pseudo-Nambu-Goldstone bosons that have spontaneously broken the global Peccei-Quinn (PQ) symmetries at very high energies. Due to the approximated symmetry shifts, the ALPs are naturally lighter compared to the electroweak or QCD particles. Future high-precision experiments may be able to find ALPs that have masses that are well below the GeV scale, but future high-energy lepton and hadron colliders may also be able to search for the heavier
ALPs. This particles are known to have very rich physical phenomenology at the targeted high- and low-energy collider experiments. Therefore, this establishes them as the prime targets for the future experiments that are aimed at the discovery of new physics that goes beyond the known and widely accepted Standard Model (SM) of particle interactions. In this work, We are investigating the possibility of detecting this new kind of particles via the charged and neutral current processes: $e^{-}\ p \to v_e\ j\ a_x$, $e^{-}\ p \to e^{-}\ j\ a_x$ for channels WW and $\gamma\gamma$, ZZ and γZ respectively and with further decay $a_x \to \gamma\gamma$ at future $e^{-}\ p$ colliders. Furthermore, we are also providing possible constraints on the available couplings $g_{a\gamma\gamma}$, g_{aWW}, $g_{a\gamma Z}$ and g_{aZZ}.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / 6

Probing Axion-Like Particles at LHC

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[2] *Indian Institute of Science Education and Research*

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Axion-like particles (ALPs) are well motivated new particles that serve as candidates of beyond the Standard Model studies (BSM). In this work, we propose to probe the ALPs through p p ⟶ a j j at the Large Hadron Collider at energy 14 TeV. The considered ALP production is both t-channel and s-channels. We demonstrate that we could provide constrains the effective coupling strength between ALPs and electroweak bosons (W ±, Z, ɣ) in a mass range Ma well below 500 GeV. Using χ2-squared analysis both on cross-sections and also on distributions, we aim to improve on the previously calculate bounds to better constrain the coupling strengths of ALPs with electroweak bosons at LHC for channels W W, ɣɣ, ZZ and Zɣ respectively and with further decay a ⟶ ɣɣ while considering the available couplings gaɣɣ , gaWW , gaɣZ and gaZZ.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics of Condensed Matter and Materials Track 1 / 7

Effects of annealing time on structural, morphology, and optical properties of Zinc oxide nanoparticles prepared via sol-gel method

Authors: Tebogo Selema[None]; Dieketseng Tsotetsi[None]; Thembinkosi Malevu[None]

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In this study, Zinc oxide (ZnO) nanoparticles were synthesized using the sol-gel method, followed by annealing at 550 oC for different time intervals (30 min, 1 hour, and 1 hour 30 min) to investigate the effect of annealing time on the structural, optical and morphological properties of ZnO nanoparticles. X-ray diffraction (XRD) analysis confirmed the formation of a crystalline hexagonal wurtzite ZnO structure, which was observed to be more prominent with an increase in annealing time, specifically at 1 hour 30 min. UV-Vis spectroscopy analysis revealed an improved absorption band with a wavelength of 365nm, which was redshifted compared to other prepared samples. Additionally, photoluminescence (PL) quenching was observed for the annealed samples, indicating charge transfer that is favorable for solar cell applications. The as-prepared sample showed high PL intensity, possibly due to self-trapped excitons recombination. This highlights the potential of modifying annealing time and its derivatives to suppress the recombination of electron-hole pairs, as higher PL intensity implies a more drastic recombination of charge carriers. Finally, the morphology of the prepared samples was studied using scanning electron microscopy (SEM), revealing a progression of ZnO morphologies from clustered to nanorod and flower-like structures. Overall, the results suggest that annealing time is a crucial parameter in the synthesis of ZnO nanoparticles, and that optimized annealing conditions can improve their structural, optical, and morphological properties for potential use in solar cell applications

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

Msc

Poster Session 2 / 8

Design and Fabrication of a Plastic Biogas Digester for the Production of Biogas from Cow Dung

Author: KeChrist Obileke[1]

Co-authors: Sampson Mamphweli [2]; Edson Meyer [3]; Makaka Golden [3]; Nwabunwanne Nwokolo [3]

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Biogas digester dimensions and materials of construction are important factors of consideration during the design and fabrication phase. &e aim of this study is to provide a detailed analysis of the design and fabrication of a 2.15 m3 pilot plastic biogas digester for biogas generation. To establish this, a design equation covering the volume of the digester, inlet and outlet chambers, and digester cover plate was developed considering the shape of the digester. The digestion chamber of the biogas digester under study was fabricated using high-density polyethylene (HDPE) plastic, while the inlet and outlet chambers were constructed with bricks/cement. &e study was motivated due to some limitations such as leakage associated with previous designs. In the present study, a ventilation test was conducted after the fabrication to ensure the digester is leak free. Results obtained showed a total volumetric methane gas yield of 2.18 m3 (54.50%) and carbon dioxide yield of 1.77 m3 (44.25%) making up a total biogas yield of 4.00 m3. In addition, the percentage concentration of methane and carbon dioxide were found to be 60% and 30%, respectively. The developed plastic biogas digester has been found to be appropriate for biogas production using cow dung as substrate.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / 9

A comparison study of some structural, vibrational, elastic and electron spin resonance properties of bulk- and nano-sized particles for ZnxCo1-xFe2-xAlxO4 ferrite samples

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Corresponding Author: masukusizwee@gmail.com

A comparison study of nanosized ZnxCo1-xFe2-xAlxO4 (x = 0, 0.2, 0.3, 0.4, 0.5, 0,7, and 0.9) and bulk counterparts obtained by annealing at 1000 0C for 3 hours is presented. X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and Raman spectroscopy studies confirmed the formation of cubic spinel structure for both the as-prepared and annealed samples. The as-prepared particle sizes range from (5 − 13 nm) while the annealed sample sizes range from (58 -62 nm). Annealing the nanoparticles at high temperatures reduces vacancies at lower concentrations ($x \leq 0.4$) of Zn and Al. On the FTIR data, the difference in absorption bands at $x > 0.4$ of the sample with nanoparticles decreases with an increase in dopants concentrations and they are lower than their bulk counterparts. The Raman mode associated with the vibration on the A-site is strongly affected

by the site preference and the reduction of vacancies on this site. ESR and magnetization measurements reveal a reduction in magnetization with increasing particle size.

Apply to be considered for a student ; award (Yes / No)?:

YES

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / 10

Optimization of the Performances of a Silicon Solar cell using a Non-uniform Doping Distribution

Author: Kapim Kenfack Abraham Dimitri[1]

Co-authors: Thantsha Nicolas Matome [1]; Msimanga Mandla [1]

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Despite several techniques of optimization of the yield of a solar cell, we remark that the use of a non-uniform doping distribution has not yet been explored. This work studies the effect of a non-uniform doping profile, on the output electrical power of a silicon solar cell. The uniform doping profile commonly used in conventional solar cells is replaced by a Gaussian doping distribution. The new doping profile leads to a nonlinear continuity equation that is solved using the Tri Diagonal Matrix Algorithm (TDMA). The simulations made under standard test conditions on the output electrical parameters reveal that, the Gaussian doping profile increases the leakage photocurrent at the edge of the solar cell and reduces the photogeneration process of the minority carriers in the solar cell. Additionally, by varing the doping concentration at the top surface and back contact of the solar cell, to vary the parameters of the Gaussian profile, the solar cell achieve an electrical power and efficiency of about 50 mW/cm2 and 50% respectively.

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 1 / 12

Synthesis of Mn-rich transition metal carbonate precursors as cathode materials for lithium ion batteries: Carbonate co-precipitation method

Authors: Mogahabo Tebogo[1]; Noko Ngoepe[2]; Clifton Masedi[3]; Phuti Ngoepe[2]

[1] *Black*

[2] *University of Limpopo*

[3] *Co-supervisor*

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Synthesis of Mn-rich transition metal carbonate precursors as cathode materials for lithium ion batteries: Carbonate co-precipitation method
Tebogo Morukuladi, Noko Ngoepe, Clifton Masedi and Phuti Ngoepe
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Abstract
The synthesis of NMCCO3 precursors for lithium and manganese rich materials was carried out via the co-precipitation method. Co-precipitation method is a widely used process in various applications to carry down by precipitate of substances normally soluble under the conditions employed. For this study, carbonate co-precipitation was used to synthesize our materials using the continuous stirred tank reactor (CSTR). The advantage of using carbonate co-precipitation is that most of the transition metal cations remains in the divalent oxidation state. The intensions of this study were to investigate the electrochemical properties for Mn-rich NMC's. After the synthesis of NMCCO3 precursors, tap density was measured, morphology, particle size distribution and XRD's were determined. A particle size distribution of 9.7 μm was observed, while the morphology shows secondary particles of the material. This findings implies that layered Mn rich LiNMCO2 is so far a good material for cathodes in lithium ion batteries.
Keywords: Tap density, Morphology, Particle size and XRD's.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 1 / 13

Ball Milling synthesis and characterization of highly crystalline TiO2-ZnO hybrids for photovoltaic applications

Author: Thembinkosi Malevutd[1]

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In this work, Ball Milling is investigated as a viable synthesis method for highly crystalline TiO2-ZnO composites. The composites were verified using various standard techniques. XRD measurements confirmed the presence of hexagonal wurtzite ZnO and tetragonal TiO2 nano particles. Both XRD and transmission electron microscopy show a mean crystallite size between 12.7 and 15.0 nm. The blend compatibility of the two oxides was investigated by varying the molar ratio of ZnO from 0 to 30%. It is apparent that the morphology compatibility of ZnO and TiO2 plays a significant role in the performance of the final device. The composite specific surface area is seen to increase with ZnO doping. UV-Vis measurements show that its band gap decreases from 3.281 to 3.221 eV. UV-vis further demonstrated a red-shift of TZHO absorption band which enhances the ability of hybrids to absorb in the visible wavelength range. Scanning electron microscopy suggests that TiO2 and ZnO are morphologically well-matched, and can be used as the electron transport layer in a blended perovskite solar cell. A maximum efficiency of 8% was measured on the PSC with 30% ZnO with Isc=18.4 mA, Voc=0.69 V, and FF=0.65. This efficiency is comparable for PSCs with the hybrid oxide synthesized using other methods, showing that Ball Milling is also a viable method.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 1 / 14

Investigation of xanthate, dithiocarbamate and triazine collectors adsorptions on sperrylite and platarsite (100) surface: A DFT-D3 calculations

Authors: Bradley Nemutudi[1]; Sophia Pikinini[2]; peace prince mkhonto[1]; Belinda McFadzean[3]; Xingrong Zhang[4]; Phuti Ngoepe[1]

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The separation of valuable minerals from the gangue minerals is still a challenge, in particular the extraction of arsenides platinum group minerals (PGMs) such as sperrylite and platarsite. It has been reported that the flotation of PGMs resulted in low recovery when using traditional xanthates. This was owed to the report that the arsenides PGMs minerals are not amiable to flotation, and therefore new collectors are required. The triazine collectors are promising reagents for mineral flotation and have not been given much attention in minerals processing. In this study, we used density functional theory with dispersion correction to perform the adsorption of sodium normal butyl xanthate (SNBX), sodium normal butyl dithiocarbamate (SNBDTC) and 2,6-dithio-4-butylamino-1,3,5-triazine (SDTBAT) on sperrylite and platarsite (100) surfaces. It was observed that the collectors preferred to bridge on surface As and Pt atoms through the S atoms on sperrylite, while on platarsite they adsorbed though mono-dentate between S atom on Pt atom. Furthermore, it was found that the adsorption energies were in the order: SDTBAT > SNBDTC > SNBX, indicating that the SDTBAT had strong exothermic adsorption on sperrylite and platarsite. Interestingly, the collectors were more exothermic on sperrylite surface than platarsite. Importantly, it was found that the triazine collector had strong adsorption than the xanthate and dithiocarbamate, which depict a promising replacement of xanthate and dithiocarbamate collectors. Therefore, these results have identified well performing collector (triazine) to improve the recovery of PGMs.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Theoretical and Computational Physics / 15

How to be an orthodox quantum mechanic

Author: Geoff Beck[1]

[1] *University of Witwatersrand*

Corresponding Author: geoffrey.beck@wits.ac.za

Quantum mechanics, like any scientific theory, has a prevailing orthodoxy for its interpretation. However, due to the abstract nature of the formalism, interpretation of quantum theories is especially contentious. In this work we attempt to quantify the quantum orthodoxy via a systematic survey of popular graduate and undergraduate textbooks on the subject. In so doing, we determine the fundamental epistemic and ontological commitments that form the bedrock of the modern orthodoxy. We then examine how these commitments are linked to several open problems in quantum foundations.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Nuclear, Particle and Radiation Physics / **16**

Health Risk Assessment of Toxic Heavy Metals in Irrigation Water, Rustenburg

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Several water sources and their state in Africa are a major concern due to mining, industrial, and other anthropogenic sources. Water is essential to life and healthy living, and also serves as home to various species of household edible fishes. Unfortunately, its contamination has led to significant deaths resulting from diseases associated with the consumption of contaminated water. Globally, toxic heavy metals are among the numerous contaminants associated with water pollution. In this study, toxic heavy metal concentration in irrigation water used in Rustenburg was measured using inductively coupled plasma-mass-spectrometry, and its associated carcinogenic and non-carcinogenic health risks were assessed. The measured concentration of toxic heavy metals in sampled water ranges from ND (not detected) to 1.20×10-04, 1.00×10-05 to 4.00×10-04, ND to 1.24×10-02, 1.20×10-04 to 1.84×10-02, ND to 5.47×10-02, 1.30×10-04 to 2.75×10-02, and ND to 1.12×10-01 for Cd, Pb, Zn, Cu, Ni, Co, and Fe respectively, with mean values of 6.24×10-05, 2.33×10-04, 4.15×10-03, 8.68×10-03, 3.37×10-03, 3.33×10-03, and 5.99×10-02. Non-carcinogenic risk resulting from dermal contact and ingestion of toxic heavy metals in water for adults and children shows no apparent risk to exposed populations because hazard quotient and hazard index values are less than 1. Estimated carcinogenic risk due to dermal contact and ingestion of toxic heavy metals were also less than 10-6, indicating negligible carcinogenic risk, thus making the sampled water safe for agricultural and domestic use for dwellers.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 1 / 17

A new 3 MV TandetronTM accelerator at iThemba Laboratory for Accelerator Based Sciences (iThemba LABS)

Author: Christopher Mtshali[1]

Co-authors: Zakhelumuzi Khumalo [1]; Mandlenkosi Msimanga [2]; Nametso Mongwaketsi [1]; Morgan Madhuku [1]; Dirk Fourie [1]; Collin Doyle [1]; Gassan Darries [1]; Caswell Pieters [1]; Lebogang Kotsedi [1]; Ntombizonke Kheswa [1]; Phillip Sechogela [1]; Mlungisi Nkosi [1]

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iThemba LABS hosts a number of research accelerators. The latest acquisition is a 3 MV TandetronTM accelerator that replaced the 51-year-old 6 MV CN Van de Graaff accelerator. The majority of the application area is dealing with materials research. The machine was installed and commissioned in 2017 by High Voltage Engineering Europa B.V. (HVEE) at the Tandetron Laboratory. The system is capable of accelerating charged particles to MeV energies from three ion sources; the Cs sputter source for heavy ions, and two Multicusp ion sources for helium ions and protons. The main purpose of the TandetronTM machine is to conduct research in ion beam analysis (IBA) and low-energy astrophysics research projects. It is connected to the experimental section via 90o analyzing and switching magnets, directing the beam of charged particles into the target chambers. There are currently two active beamlines dedicated to (1) solid-state physics techniques, such as RBS and ERDA, and (2) nuclear microprobe-based techniques, such as PIXE and proton beam writing. Another beamline, currently being commissioned, is for astrophysics-related projects. The available ion sources are capable of delivering high-intensity beams of 200 eμA and 25 eμA for protons and helium light ions, respectively, while delivering 150 eμA for heavy ions, at a maximum terminal voltage (3 MV). This demonstrates a huge potential in materials research areas such as ion implantation, radiation hardness testing, and shielding studies. Important features of the accelerator and energy calibration are discussed.

Apply to be considered for a student ; award (Yes / No)?:

no

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 2 / 18

Kinetic analysis and dosimetric features of thermoluminescence of tanzanite

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Tanzanite is a rare gem mineral of high commercial value and sensitive to optical and thermal stimulation of luminescence. Kinetic analysis and dosimetric features of thermoluminescence from tanzanite are reported. A glow curve measured at 1 ℃/s following beta irradiation to 70 Gy reveals a high intensity peak at 74 ℃ and two distinct lower intensity peaks at 138 and 186 ℃. The peaks

are respectively referenced as I, II and III. The dependence of the peak position on partial heating and irradiation dose shows that all peaks are of first order kinetics. Kinetic analysis of peak I was carried out using various analytical methods including initial rise, whole glow peak, curve fitting, phosphorescence, phosphorescence area and variable heating rate. The activation energy was averagely evaluated as 0.83 eV. The dose response of all peaks is sublinear from the supralinearity index analysis. Phosphorescence measurement at room temperature shows that peak I is affected by thermal fading unlike peaks II and III which are stable.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Nuclear, Particle and Radiation Physics / **19**

The Decline and Fall of Nuclear β- and γ-Vibrations

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The conjecture of Bohr and Mottelson that the lowest Kπ = 0+ and Kπ = 2+ rotational bands in deformed nuclei could be identified as “vibrations” of the quadrupole shape, turns out to be fallacious. The vast amount of current experimental data shows that the Kπ = 0+ rotational bands are 2p-2h states and that the Kπ = 2+ rotational bands are due to the energy being lowered by the nucleus favouring triaxiality and rotating about its intermediate axis.
The experimental data mitigates against current, but still fashionable, nuclear models such as the Interacting Boson Model (IBM) and interpretations involving phonon excitations.
It is significant that the deformed mean-field and single particle behaviour is valid all the way up to fission.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 1 / **20**

Alloying on β2-ordered FeAl with Ru and Ir for ductility enhancement: A cluster expansion and MD approach

Author: CHRESTINAH MKHONTO[1]

Co-authors: Phuti Ngoepe [2]; Hasani Chauke [2]

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[2] *University of Limpopo*

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Intermetallic iron aluminides alloys of Fe3Al and β2-ordered cubic FeAl structure amongst other various compounds of transition metals and aluminium compositions have been of interest to researchers for application in different industries to increase corrosion-resistance for high temperature application steel coating. The FeAl compound exists between 35-50 % of aluminum concentrations. This alloy possesses far much better oxidation and corrosion resistance and hardness qualities than the Fe3Al. Their long-range-ordered superlattices, which minimizes dislocation and diffusion at increased temperatures make them desirable for high temperature applications. We have employed the cluster expansion (CE) technique to construct the stability phase diagrams of Fe-Ru/Ir-Al ternary systems for stable compositions identification, Monte Carlo (MC) to determine the temperature needed to stabilize the system and ab-initio approach to predict the mechanical and dynamical properties using LAMMPS code. The cluster expansion results showed that the Fe1-XRuXAl ternary alloy has no thermodynamically stable compositions due to positive enthalpies of formation values, while the Fe1-XIrXAl alloy has values that are marginally above 0 eV. It was observed that the Fe1-XIrXAl system has three thermodynamic stable structures; the stability of the system increases with Ir concentration until the Fe:Ir reaches an equiatomic composition and began to decrease. Hence, FeIr2Al3 system was found to the most thermodynamically stable composition. Our findings showed that doping the β2-FeAl with Ru and Ir significantly enhanced the hardness and ductility for high-temperature application for steel-It component coating.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics of Condensed Matter and Materials Track 1 / 21

Characterization of defects in ZnO implanted with Ar+ using positron annihilation technique.

Author: Musawenkosi Khulu[1]

Co-authors: Morgan Madhuku [2]; Thulani Jili [1]; Cebo Ndlangamandla [1]; Phumlani Zipho Ngcobo [1]

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ZnO (wurtzite) samples were implanted with Ar+ ions to generate intrinsic defects within the ZnO samples at fluence range from 1 x 1015 to 3 x 1016 ions.cm-2. Doppler broadening of the annihilation curves were obtained to determine S-parameters which are used to characterize the defects. S-parameters are 0.35795, 0.35809 and 0.39025 for the lowest to the highest fluence, respectively. X-ray diffraction method was employed to determine any structural damage or phase change during the implantation. Positron annihilation spectroscopy shows the formation of anion point defects. Optical absorption measurements suggest the presence of F aggregate centres at 300.0 nm (4.14 eV). Theoretical calculations of the annihilation curves, based on local density approximation as well as generalized gradient approximation, were obtained. Theoretical results compare well with experimental results. Positron annihilation measurements are also correlated with optical absorption results on Ar+ ion implanted zinc oxide crystal.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics of Condensed Matter and Materials Track 1 / 22

The capability of cerium (Ce) to improve the magnetic properties of Nd2Fe14B magnet: A computational approach

Authors: Mphamela Enos Baloyi[1]; Phuti Ngoepe[1]; Hasani Chauke[1]

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Neodymium-based permanent magnets (Nd2Fe14B) are the potential permanent magnets for use in various applications such as wind turbines and electric vehicles due to their high magnetic field strength and resistance to demagnetisation. However, they suffer from low operating temperatures below 585 K and poor mechanical and vibrational properties. In this study, we investigate the effect of Ce on the magnetic and mechanical properties of Nd2Fe14B magnets using the ab initio density functional theory (DFT) approach. The NdCeFe14B magnets are found to be thermodynamically and mechanically stable. The alloying of Nd with Ce improves the stability and magnetic strength of Nd2Fe14B permanent magnets. The findings will provide insight into the future development of permanent magnetic compounds with good magnetic strengths.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Astrophysics & Space Science / 23

Assessment of wildfire emissions using satellite and reanalysis data: A review

Authors: Lerato Shikwambana[1]; Mahlatse Kganyago[2]; Paida Mhangara[3]

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Wildfires are among the major and prevalent environmental disturbance agents of our time and affect human health, the infrastructure and the earth-atmosphere mechanisms. Wildfires can be ignited naturally by lightning or humans, either accidentally or to accomplish management objectives such as clearing and reduction in fuel loads. Wildfires are unique in themselves as they are driven by various factors such as fuel type, topology, and meteorology. In this work we highlight studies that have observed emissions of gases and aerosols from different regions globally and how they compare. The work further looks at the spatial distribution of black carbon (BC), carbon monoxide (CO) and smoke from wildfires. The emissions of BC, CO, and smoke are retrieved from the Modern-Era Retrospective Analysis for Research and Applications version 2 (MERRA-2), Sentinel-5P and Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations (CALIPSO), respectively. Lastly, in this

work we report on the relationship between the meteorological parameters, vegetation conditions and emission parameters using the Pearson's correlation. Overall, this work demonstrates the value of multisource remotely sensed data in characterising long-term wildfire patterns and associated emissions.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 2 / 24

Effect of polymer coating on the calcium ferrite nanoparticles for biomedical applications

Authors: Wendy Mdlalose[1]; Seipati Mokhosi[2]

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Magnetic nano ferrites with superparamagnetic behaviour have attracted great interest in biomedicine. When these nano ferrites are coated, surface oxidation and aggregation can be reduced, enhancing their stability. In this work, CaFe2O4 nanoparticles (NPs) were synthesized through a glycol-thermal reaction method and coated with polymers viz: chitosan (CH) and polyvinyl alcohol (PVA) to yield CH–CaFe2O4 and PVA– CaFe2O4 NPs, respectively. Both naked and coated NPs were characterized by X-ray diffraction (XRD), which revealed the configuration of the cubic spinel structure. The crystallite sizes for CaFe2O4, CH–CaFe2O4 and PVA–CaFe2O4 NPs are 6.13 nm, 5.61 nm and 6.36 nm, respectively. Transmission electron microscopy (TEM) and scanning electron microscopy (SEM) showed spherical morphology for all NPs. The hydrodynamic size distribution observed for naked NPs (92 ± 4 nm) increased upon coating with CH and PVA to 169 ± 4 nm and 151 ± 14 nm, respectively. Magnetic analysis using a vibrating sample magnetometer (VSM) revealed that all NPs exhibited superparamagnetic behaviour with saturation magnetizations of ˜38.52 emu/g, 11.27 emu/g and 37.73 emu/g for CaFe2O4, CH–CaFe2O4 and PVA–CaFe2O4 NPs, respectively. Further, in vitro cytotoxicity profiling using the MTT assay showed that CH-CaFe2O4 NPs are well tolerated by the human embryonic (HEK 293) cell lines at concentrations of up to 100µg/ml. This trend was also observed in the human cervical cancer (HeLa) cell lines. Moreover, in HeLa cell lines, there was no significant toxicity with all NPs. The lowest reported viabilities were 67.6% at the high 400 µg/ml concentration for CH-CaFe2O4 NPs. Polymer coating seemed to result in improved cytotoxicity profiles. To this end, calcium ferrites and their polymer-coated derivatives can be explored as potential nanocarriers in gene and drug delivery.

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No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

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Poster Session 1 / 26

Effect of Co on structural, stability and ductility of Fe5Ni4S8 (P4_2/nmc): Cluster expansion method

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Co-author: Mofuti Abram Mehlape [1]

[1] *University of Limpopo*

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Pentlandite ((Fe,Ni)9S8) is a primary source of nickel and is largely found in the Merensky reef which host the largest amounts of base metal sulphides (BMSs) and is also known to host platinum group elements (PGEs). Palladium and rhodium are the PGEs contained mostly in pentlandite, cobalt (Co) is also one of the metal found in association with pentlandite. The milling of pentlandite prior to flotation has presented challenges which are associated with its brittle nature. In the present study the cluster expansion (CE) method was used to predict the stable (Fe,Ni)9S8 pentlandite structure. The Fe5Ni4S8 pentlandite compound was found as the most stable structure, which possessed a space group of P4_2/nmc. Furthermore, Fe5Ni4S8 was doped with Co using cluster expansion and found that the (CoFe4Ni4S8, Fe4CoNi4S8 and Fe5Co2Ni2S8 i.e Co doped at Fe(O), Fe(T) and Ni(T)) composition were the most stable. The calculated Bulk to Shear modulus ratio (Pugh's ratio) of CoFe4Ni4S8, Fe4CoNi4S8 and Fe5Co2Ni2S8 system were greater than 1.75, which showed that Co increased the ductility of Fe5Ni4S8 (P4_2/nmc). Additionally, the symmetry of Fe5Ni4S8 (P4_2/nmc) remained tetragonal after Co doping.
Moreover, the heats of formation for Co doped systems was greater than of un-doped Fe5Ni4S8 (P4_2/nmc), suggesting that Co increased the thermodynamic stability of pentlandite.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 1 / **27**

Effect of temperature on β-TiCl3 medium

Authors: Andile Mazibuko[1]; Hasani Chauke[1]

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The magnesiothermic reduction of titanium tetrachloride (TiCl4) results in the formation of titanium subchlorides such as titanium trichloride (TiCl3) and titanium dichloride (TiCl2). However, this process occurs extremely fast and it is not suitable for the development of a continuous reduction process. In this study, classical molecular dynamic calculations were performed to understand the influence of temperature on the TiCl3 (β-TiCl3) structure (using rigid ion and shell model) with P63/mcm space group, employing the DL_POLY code. It was found that for the rigid ion model chlorine diffuses at 300 K. The entropy and Gibbs free energy was used to deduce the behaviour of atoms and the spontaneity of the structure. Positive entropy is noted at 600 K – 700 K for the rigid ion model and at 700 K for the shell model, indicating possible melting. In addition, the system was also observed to be spontaneous (favourable) for both models at 50 K – 2000 K. The results of this study give us more insight into the TiCl3 medium as a potential medium for evaluating titanium.

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Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Theoretical and Computational Physics / 28

Black holes and nilmanifolds

Author: Alan Cornell[1]

Co-authors: Deandrea Aldo ; Anna Chrysostomou [1]

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Corresponding Author: alanc76@gmail.com

We investigate whether quasinormal modes can be used in the search for signatures of extra dimensions. To address a gap in the literature, we focus on negative Ricci curvature extra dimensional spacetimes. Starting with a product space comprised of a four-dimensional Schwarzschild spacetime and a 3-dimensional nilmanifold, we study the scalar perturbations. The geometry can be characterised as the effective potential of a squared mass-like term. We then compute the corresponding quasinormal frequency spectrum and determine constraints on this possible extra-dimensional observable from gravitational-wave considerations.

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No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Theoretical and Computational Physics / 29

Weak Gravity Conjecture for dilaton de Sitter black holes in extra dimension

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Co-authors: Alan Cornell [2]; Aldo Deandrea [3]; Anna Chrysostomou [4]

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The Weak Gravity Conjecture (WGC) is a theoretical conjecture that relates gravity to other forces within the framework of an Effective Field Theory (EFT). One of the primary motivations behind the WGC is to provide a kinematic constraint on the decay of extremal black holes. This kinematic constraint arises from the notion that the black hole must decay to states that are incapable of forming new black holes. As such, objects that would give rise to naked singularities, which are prohibited under the Weak Cosmic Censorship hypothesis, must be particles.

In this talk, we consider charged black hole solutions of the Einstein-Maxwell-dilaton theory in de Sitter space. Our investigation focuses on examining the location and existence of horizons as a function of the parameters for mass (M), charge (Q), and dilaton coupling strength (α) in the context of extra-dimensional spacetimes, and investigating possible modifications of the Weak Gravity Conjecture in the extra-dimensional spacetimes. In n-dimensions, for a spatial value of $\alpha_c^2 = \frac{(n-3)^2}{(n-1)}$, we observe that there is a new extremality condition, or a new WGC bound. Moreover, we find that, because of the complexity of the metric for $\alpha < \alpha_c$, the extremal case is not achieved for the de Sitter space.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics for Development, Education and Outreach / **30**

Evaluating Essential Skills

Author: Derek Fish[1]

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Operating from the University of Zululand, Unizulu Science Centre (USC) had been running face to face matric workshops for 25 years, presenting practicals and sharpening skills for over 200 000 matric science students. The 2020 lockdown presented a dilemma: matrics needed assistance more than ever, but schools were closed and large gatherings impossible. USC piloted a unique offline, digital video project (Essential Skills for Matric Science – ES) which was reported on at the 2021 SAIP conference. USC worked to convert a 4 hour contact workshop into first 8, then later 16, one-hour videos, highlighting the essential skills for Matric Science Paper 1 – the physics paper. While these videos were made available on the internet (via the SAIP website) for download or streaming, they were physically distributed on memory sticks to teachers, along with an accompanying workbook. Local industry funding initially and then further SAIP funding (with support from Allan Gray) saw 100 000 booklets printed and 2 000 memory sticks manufactured over the next three years. These have been distributed to schools in all nine provinces and also used as the basis for teacher training, especially by the SAIP. The framework for ES has already been used to generate a similar tool for Life Science and Chemistry. Videos and booklets for Mathematics are under development.

Looking back over three years, it is essential to try to measure the impact of this project and how it can be made more effective for the future. A simple evaluation tool was used with key stakeholders who had been very involved in ES during this time, to gather their inputs on the ES project, how well it had worked and what could be improved. A synthesis of their responses will be presented to inform an evaluation of what has been achieved and what can be achieved in future. In particular the transition of ES from a distance only model (during lockdown) to a hybrid one (after lockdown) will be discussed. The inputs of the Physics Education Group members (many of whom had personal experience of ES) will be much appreciated.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics for Development, Education and Outreach / 31

Studying the other 95 %: free-choice learning evaluation for Physics.

Author: Derek Fish[1]

Co-author: John Falk [2]

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For tens, if not hundreds of thousands of years, learning was widely understood to be an everyday occurrence, something people did to support their needs and interests. In this world, most people, most of the time, controlled their own learning. Learning was active, supported by observing others, doing and practicing. Learning happened in pairs or in small groups typically supported by peers and skilled practitioners. Importantly, evidence of "successful learning" was not something judged by others but something demonstrated through competent actions and deeds in real life. This natural, choice-driven form of learning is what is called free-choice learning.

Then, roughly 150 years ago everything changed. Learning became increasingly thought of as something that only happened in schools. Learning came to be seen as an institutionalized and "professionalized" process, initiated and directed by experts. To say the word learning to someone conjured up ideas of a passive and mass-produced kind of activity where information was transmitted to large groups of "students" through lectures and textbooks, where the goal was passing tests rather than having the knowledge, skills and habits of mind necessary for solving real life problems.

Over the next 50 years we will be going back to the future! As the public's need to learn expands, so too will the public's perceptions of what it means to learn. Freed from the tyranny of equating learning with schooling, the public will find themselves engaged in an ever increasing array of free-choice learning experiences across an ever-wider array of platforms. Already, most people learn most of what they need and want to know through free-choice learning. Every year, schools and universities provide a smaller and smaller fraction of the public's true education.

Only 5% of our lifetime learning takes place inside the classroom, lecture hall or laboratory. For over three decades the Institute for Learning Innovation (ILI) has studied the other 95 %:- investigating learning, learners and their various motivations. Dr John Falk has led this free-choice learning research in the ILI and worldwide for over 50 years. Dr Derek Fish is currently spending a year working with Dr Falk and the ILI on a Fulbright Scholarship.

The "Physics Education" track has changed over the years and now covers "Physics for Development, Education and Outreach." While the traditional tools of Physics Education Research (PER) are well known to this group, development and outreach take place outside the classroom and cannot be evaluated in the same way. Dr Falk and Dr Fish will share the tools and practices of evaluating free-choice learning activities which will assist participants in this Track in broadening their horizons from Physics for Education only to Physics for Development, Education and Outreach.

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No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Astrophysics & Space Science / 32

Pulse fitting and spectral analysis of Fermi -GBM short GRBs with known redshift and comparisons with magnetar giant flares

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Short gamma-ray bursts (SGRBs) are energetic impulses with emissions that last for less than 2 s and have a hard spectra. They are cosmological entities and they originate from compact binary mergers like binary systems. Moreover, there is evidence that they are also tied to gravitational wave events after the detection of GRB170817A. However, these properties are not unique to them. There are other short gamma-ray transients that posses similar properties called magnetar giant flares (MGFs). They however, originate from magnetars in our galaxy or in nearby star-forming galaxies. When MGFs are observed at great distances only their prominent peaks are observed hence can be confused with the cosmological SGRBs. Typically, their spectra has a prominent peak which is then followed by prolonged fading pulses. Without the detection of the oscillating fading phase, the distinction between SGRBs and MGFs is hindered if the redshift is unknown. MGFs typically have isotropic energy in the range $10^{44} - 10^{47}$ erg whilst SGRBs are highly energetic with isotropic energy around 10^{52} erg. In this work, both transients with prominent peaks were fit with the Norris function to get their pulse rising times at varying energy ranges and the goodness of the pulse fit was measured with the χ^2 value. Their pulse rising times are utilised to make a distinction between the two transients. MGFs posses pulse rising times that last for hundreds of ms whilst for SGRBs its a few ms. Moreover, spectral analysis was performed in the energy range 10 kev - 40 MeV and data fitting was achieved with the Comptonised and Band model for the brightest detector for each SGRB. The significance of these fits was determined with the Cash Castor-statistics. The bursts utilised in the spectral analysis have known red-shift and were detected by the Fermi-GBM instrument.

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Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics of Condensed Matter and Materials Track 1 / 33

Modified ZrO2 layer on ZIRLO to prevent Hydrogen Pick Up.

Authors: Sinoyolo Ngongo[1]; Arno Janse van Vureen[1]; J.H Neethling[1]; V.V Uglov[2]

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Zirconium alloy is the main physical barrier between the coolant system and the fuel cell1. Its principal role is to keep the radioactive products produced during fission process (which is the power source in the nuclear reactor) contained in the fuel pin1. One of the problems in the nuclear industry is hydrogen absorption by zirconium alloys during operational and loss of coolant accident environment. This hydrogen diffusion into the fuel tube (zirconium alloys) leads to formation of brittle zirconium hydrides2. Theoretical predictions by Youssef and co-workers3 indicated that by doping the oxide layer on the zirconium alloy with chromium, the solubility of hydrogen in ZrO2 is greatly decreased which reduce the pick-up of hydrogen by the zirconium fuel tube.

In this study, compression plasma flow (CPF) was used to produce a chromium doped, oxidized ZIRLO surface layer. CPF is generated by quasi-stationary plasma accelerators with their own magnetic field. Such plasma flows are characterized by long life-time (about 100 μs) and high energy density absorbed by the target (from 10 to 100 J/cm2). When CPF interacts with the surface, the top layer is melted and a mixing process takes place in the layer. If a metal coating is deposited on the surface of the treated sample, the CPF impact will provide mixing of both coating and the substrate. A chromium coating with a thickness of 1 μm was deposited on the oxidized ZIRLO surface. The CPF treatment was done in a nitrogen atmosphere (400 Pa pressure). The chromium alloyed ZIRLO samples were sectioned using a diamond wire saw and mounted on a stub. A Helios NanoLab FIB SEM was used to cut transmission electron microscopy lamellae from specific areas of interest. The TEM lamellae were investigated in a JEOL 2100 LaB6 TEM operated at 200 kV.
The results of this investigation indicated that the alloying process of the oxide layer by the CPF method was successful. The thickness of the Cr modified oxide layer is about 2 μm. The hydrogen pick up investigation of the modified sample was carried on the special gas Reaction Controller complex. Results of hydrogen desorption from the chromium doped oxidized ZIRLO surface layers were found to be in agreement with the theoretical predictions by Youssef and co-workers3. Comparing the unmodified and modified sample the hydrogen desorption decreased by a factor of 26.
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2. Motta, A.T., Chen, L.Q. (2012) J. Min. Met. Mater. Soc. 64 (12).
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Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Applied Physics / 34

Effect of concentrator geometry on wind velocity augmentation

Author: Chipo Shonhiwa[1]

Co-authors: Golden Makaka [1]; Patrick Mukumba [1]; Ngwarai Shambira [1]

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South Africa is experiencing acute energy shortages leading to prolonged load shedding. Renewable energy can be a solution to this energy problem. From the renewable energy resources, wind has a great potential of increasing the energy mix and help in abatement of climate change. It is one of the fastest growing energy technologies that can substitute fossil fuels in electricity production. Most wind turbines that are available on the market need wind speeds above 5 m/s to produce meaningful electricity. Regrettably some areas don't have such high wind speeds. Several researches have been done in coming up with techniques for improving wind turbine power output in low wind speed areas. Concentrator Augmented Wind Turbines (CAWTs) have been proved to increase the effectiveness of the wind turbines in low wind speed areas by increasing the wind speed upstream of the turbine. However, the effect of concentrator geometry on the velocity augmentation capability of the concentrator is not clearly understood to enhance the designing of competitive CAWTs. This study investigated the effect of concentrator geometry on velocity augmentation. Computational fluid dynamics was used for the investigations. A model was analysed in ANSYS Fluent® software and validated by experiments. The performance of 45 concentrators was investigated in terms of concentrator efficiency and velocity augmentation ratio (*vr*). The concentrators had the same outlet radius and their geometry was varied by changing the concentrator length (*L*) and the outlet radius (*R*). It was observed that the changes vr was affected by the change in both the *L* to *2R* ratio (*Lr*) and the difference between inlet and outlet radii to *2R* ratio (*Rr*). As *Lr* was increased from *Lr* = 0.1,

the *vr* increased to pick at *Lr* = 0.4 and then decreased with farther increase in *Lr*. Also, as *Rr* was increased from 0.025, the *vr* increased to peak at *Rr* = 0.1 and then decreased as *Rr* was increased. It was also shown that the energy losses due to friction have more negative impact on velocity augmentation than energy losses due to large concentrator tilt angle at high *Lr* because friction on the walls occurred over a large range. From a distance L before the inlet, the wind accelerated constantly to a maximum speed at the concentrator outlet. It continued with this speed up to *0.5L* distance behind the concentrator and started to decelerate. The velocity was maximum from the concentrator centre to 80% of the outlet radius. It decreased to 0 m/s on the concentrator wall. At any distance greater than *0.1r*, the wind velocity was higher than the concentrator inlet velocity. For optimum Lr and Rr, maximum velocity was achieved at the concentrator outlet. It was concluded that when constructing a CAWT, the turbine rotor should be placed at any distance between the concentrator outlet and *0.5L* behind the concentrator and the blade tips of the turbine in a CAWT system should be at least 10% smaller than the concentrator outlet radius, for the rotor to receive wind with augmented velocity.

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No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / 35

Influence of rare-earth elements (RE = Ce, Nd, Gd) on Structural, ESR and Mössbauer spectroscopy studies of Ni0.5Co0.5RE0.03Fe0.197O4 synthesized by glycol-thermal method

Authors: T. A Nhlapo[1]; T. Moyo [2]; T. P. Mokoena [3]; S.T. Dlamini[2]; T. D Malevu[4]

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[2] *UKZN*

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Nanocrystalline Ni0.5Co0.5RE0.03Fe0.197O4 (RE = Ce, Nd, Gd) were synthesized by glycol-thermal method. X-ray diffraction (XRD) results confirm the formation of single-phase spinel ferrite. The crystallite sizes ranged from 6.29 nm to 9.41 nm which was comparable to results obtained using Williamson-Hall (W-H) method. Lattice parameters were found to vary from 8.356 Å to 8.370 Å depending on an atomic radius of a substituted rare-earth element. Large specific surface areas ranging between 120 m2/g and 160 m2/g were associated with smaller crystallite sizes. Scanning electron microscope (SEM) revealed homogeneous and clustered nanoparticles. The energy dispersive X-ray (EDS) spectra revealed the existence of nickel (Ni), cobalt (Co), iron (Fe), and oxygen (O) in an undoped sample, as well as additional characteristic peaks of cerium (Ce), neodymium (Nd) and gadolinium (Gd) were observed for doped samples. Fourier transform infrared spectroscopy (FTIR) also confirmed the formation of spinel ferrites. The electron spin resonance (ESR) results demonstrated g-values ranging between 3.10 and 3.79 which indicated strong exchange interaction between nanoparticles, type of morphology, and crystalline nature of particles. These high values make Ni0.5Co0.5RE0.03Fe0.197O4 (RE = Ce, Nd, Gd) materials suitable for applications in high-frequency devices. The Mössbauer spectroscopy results revealed the formation of broadened Zeeman lines and quadrupole-split lines as well as the presence of the Fe3+ ions at B sites in the samples.

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No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

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Poster Session 1 / 36

THE CATALYTIC ACTIVITY OF MO₂ (M= Ti, V, Mn) ON (110) SURFACE OF Na-AIR BATTERY

Authors: PERCY NGOBENI[1]; Phuti Ngoepe[2]; khomotso Maenetja[3]

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Metal-air batteries have a far higher theoretical energy density than lithium-ion batteries and are frequently proposed as a possibility for next-generation electrochemical energy storage for applications like electric vehicles and grid energy storage. The Na-air battery is an energy storage system with moderate catalytic activity in the Oxygen Reduction Reaction (ORR) and Oxygen Evolution Reaction (OER). The current study uses the Density functional theory (DFT) to develop a deeper understanding of the catalytic activity of rutile types of MO₂ for the ORR and OER in Na-air batteries. As oxygen is adsorbed on Na/MO₂ (110) surfaces, the electronic properties of several configurations (dissociated, superoxide, peroxo on Na-M, and dissociated') are examined to determine the catalytic influence towards the generation of the discharge product in Na-O₂ batteries. Using the density of states analysis, the MnO₂ system was found to be more stable than TiO₂ and VO₂ systems. These discoveries are significant for the nucleation and development of Na₂O₂ and NaO₂, as well as for understanding the reactivity of Na/MO₂ (110) surfaces.

Apply to be considered for a student ; award (Yes / No)?:

YES

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics of Condensed Matter and Materials Track 2 / 37

Fluorination of Li1.2Mn0.8O2 Cathode Material: A Computational Study

Author: Vusani Mikosi[None]

Co-authors: Kemeridge Malatji [1]; Noko Ngoepe [2]; Phuti Ngoepe [2]

[1] *Supervisor*

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Anion doping is considered an effective way to enhance the stability of Li-rich Mn-based cathode materials as it mitigates oxygen loss and enlarge the inter-slab spacing of these materials. In this study we investigate the effects of fluorine doping on Li1.2Mn0.8O2 cathode material which was constructed from Li2MnO3 that is well known for its high energy density and high specific capacity. We use the genetic algorithm within the cluster expansion to generate phases of F-doped Li1.2Mn0.8O2, and consequently determine the most stable phases. The genetic algorithm generated 78 new phases of the F-doped Li1.2Mn0.8O2 with negative enthalpies of formation indicating that the constituents are miscible. Eleven (11) of these phases are at a specific x-concentration on the ground state line of the binary diagram and are predicted to be thermodynamically stable. The most stable phase is Li1.2Mn0.8OF which lies at the position x=0.5 on the binary diagram since it has the lowest energy of formation. In addition, First-principle calculations were performed to study the structural, mechanical, and electronic properties of the most stable structure. The obtained elastic constants showed that the material is mechanically stable under the strain 0.001 as it obeys the mechanical stability criteria for triclinic crystals. The Pugh ratio predicts the material to be ductile. The density of states shows no band gap at the fermi level confirming the conductivity of the generated material. In conclusion, the addition of fluorine to Li1.2Mn0.8O2 confirms its potential in improving the issues surrounding the Li-rich Mn-based cathodes.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / **38**

Probing the Stability of Nickel Titanium Surfaces for Oxygen Adsorption: A DFT Study

Author: vukosi chauke[1]

Co-authors: David Tshwane [2]; Phuti Ngoepe [1]; Hasani Chauke [1]

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NiTi-based intermetallic compounds are known as shape memory materials and are frequently utilized in industries like aerospace, machinery, medical applications, and electronics. This is due to their structure memory effect, super elastic behaviour, high tensile strength, and biocompatibility. However, this NiTi alloy is still a contentious material due to its unstable surface and oxidation during use, more importantly, their restricted surface characteristics and adsorption process. Density functional theory (DFT) was employed in this study to investigate the surface stability and oxygen adsorption on NiTi (1 1 0) and (1 0 0) surfaces. Surface energies were analysed and it was found that the NiTi (1 1 0) surface with the lowest surface energy value is more stable than the (1 0 0) surface. In addition, oxygen adsorption was carried out on NiTi (1 1 0) surface at different adsorption sites such as the apex, bridge and hollow sites to determine the oxidation mechanism. It was found that oxygen adsorption at three possible adsorption sites and their reaction occurs spontaneously, which is attributed to the negative adsorption energy values. More importantly, the bridge site of NiTi (1 1 0) is considered the most favourable, as it has stable adsorption energy compared to other surface sites. The findings will have a good impact on the understanding of the surface stability and oxidation mechanism of NiTi surfaces.
Keywords: NiTi alloys, adsorption, surface energy, DFT

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

Hons

Theoretical and Computational Physics / 39

Insight into the effect of rhodium atom on TiN (N = 1 – 20) nanoclusters: A DFT investigation

Authors: Moeti Ramalebana [1]; Tshegofatso Michael Phaahla[1]; Phuti Ngoepe[1]; Hasani Chauke[1]

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Doping monometallic nanoclusters with other transition metal atoms have received significant attention since they can be rationally designed and integrated to achieve unique properties and functions. These properties are suitable for use in applications such as catalysis, microelectronics and nanotechnology. In this study, a density function theory approach was employed to investigate the structural and electronic properties of TiNRh (N = 1-20) nanoclusters. The calculations showed that rhodium impurity prefers the apex and mostly occupies the faces of titanium nanoclusters. The Rh doped Ti nanoclusters revealed enhanced binding energy in comparison with bare Ti nanoclusters. The relative strength displayed the shifting of the stability from N = 7 for pure Ti nanoclusters to N = 13 for Rh doped Ti nanoclusters. Furthermore, the dissociation energy showed excellent correlation with the relative stability trend. The HOMO-LUMO revealed the lowest energy gap at Ti12Rh (N=13), which correlates well with the relative stability and dissociation energy.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / 40

The Minimal load potential of elastic membranes

Author: Seyyed Abbas Mohammadi[1]

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The versatility of elastic membranes as building blocks in mechanical vibration has led to their widespread use in various fields of science and technology, including architecture and construction, medical devices, industrial applications, consumer goods, aerospace and defense, energy applications, and the entertainment industry. Their unique ability to stretch and return to their original shape has made them a crucial material for many applications. To design more efficient membranes, it is essential to study the physical properties of these structures in-depth, gaining further insight into their behavior. This study focuses on a steady state, homogeneous elastic membrane and its optimal load potential under the presence of a vertical load. By assuming a fixed amount of total load energy, we aim to adjust the vertical force to achieve the minimum load potential energy. Our goal is to find a distribution pattern for the force over the membrane that results in the lowest load potential. Mathematically, this leads to an optimization problem with an elliptic partial differential equation

as a constraint, resulting in a PDE-constrained optimization problem. It has been established that this problem has a unique solution, and for circular membranes, the optimal load can be derived analytically or in closed form. However, for membranes of general shape, a numerical method has been developed to compute the optimizer. Our numerical approaches have been demonstrated to be robust and efficient through several numerical results for non-circular membrane shapes. These results provide a distribution pattern for vertical forces that optimizes the load potential.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Consent on use of personal information: Abstract Submission:

Astrophysics & Space Science / **43**

Multi-fluid perturbations in $f(T)$ gravity

Authors: Amare Abebe[1]; Shambel Sahlu[1]

[1] *North-West University*

Corresponding Author: 33659273@mynwu.ac.za

The cosmological perturbations for a multi-component cosmic medium is investigated in the frame-work of the modified teleparallel gravity. The evolution equations of theperturbations for each component fluid are derived following the covariant and gaugeinvariant perturbations formalism. For the analysis of our results, we consider the power-law $f(T)$ gravity toy model and study the growth of the matter density fluctuations deep in the radiation- and dust-dominated epochs. We will then highlight the effect of torsion in the formation of large-scale structure formation in the universe.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 2 / **44**

Performance of the special C10 cells of the Tile Calorimeter of the ATLAS detector during Run 2 data taking period

Authors: Phuti Ntsoko Rapheeha[1]; Bruce Mellado[1]

[1] *University of the Witwatersrand*

Corresponding Author: ntsoko.phuti.rapheeha@cern.ch

The Tile Calorimeter of the ATLAS experiment at the Large Hadron Collider is a hadronic calorimeter that is designed to provide important information for the reconstruction of physics objects like hadrons, jets, tau-particles and missing transverse energy. The calorimeter also plays a role in the

identification of muons. It is a hadronic sampling calorimeter that uses scintillating tiles that are sandwiched between slabs of steel that act as an absorber. The light produced by particles traversing through the detector is transmitted by wavelength shifting fibres to photomultiplier tubes. The response of the calorimeter is calibrated to the Electromagnetic scale, which represents a basic unit in the physics object reconstruction procedures.

The performance of the special c10 cells of the Tile calorimeter is studied by their response to muons originating from $W \to \mu\nu_\mu$ events collected by the ATLAS detector during the Run 2 data taking period. The response is quantified by measuring the amount of energy deposited per unit length of each cell, in both the data and Monte Carlo simulations. The ratio of the response in data and Monte Carlo is used to quantify the calorimeter response, with deviations from unity hinting that there might be poor EM energy scale calibration in the experimental data.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / 45

Study of the Performance of Blended Mixtures of Henna and Black Plum Plants as a Co-Sensitizer in Dye-Sensitized Solar Cells (DSSCs)

Authors: Adelowo Abraham[1]; Adekunle Dauda [2]; Ojo Emmanuel[3]; Ewa Ita[4]

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[2] *National Agency for Science and Engineering Infrastructure*

[3] *Federal University of Technology Minna Nigeria*

[4] *National Agency for Science and Engineering Infrastructure NASENI Abuja Nigeria*

Solar energy is our most abundant source of renewable energy especially the use of photovoltaic material. Dye-Sensitized cells (DSSCs); a suitable photovoltaic material that has been under extensive research due to its low cost, simple preparation, low toxicity and ease of production. Hence, this research investigated the performance of two natural pigments extracted from two locally available plants [Lawsoniainermis (henna) and vitexdoniana (blackplum)] as a photovoltaic material using the modified Soxhlet technique. Three (3) blends of henna and black plum (100:0, 50:50 and 0:100) were prepared, the photo-electrochemical parameters; power conversion efficiency (η), Fill Factor (FF), Short-Circuit Current (Isc), Open-Circuit Voltage (Voc) were evaluated. The produced absorption values were 4.564, 4.004, and 4.597 respectively. The values of photo-electrochemical parameters of the three (3) fabricated cells were: FF = 47, Isc = 0.02 mA, Voc = 0.0135V, η = 0.13% ; FF = 51, Isc = 0.07 mA, Voc = 0.054V, η = 2.16 %; FF = 59, Isc = 0.05 mA, Voc = 0.0225V, η = 0.67% respectively. From the above, it is concluded that results of the blended combination of henna and black plum leaves extracts in this ratios enhanced the conversion efficiency of the DSSCs.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Theoretical and Computational Physics / 46

Quasinormal modes calculated with physics-informed neural networks

Authors: Anele Ncube[1]; Alan Cornell[2]

[1] *University of Johannesburg*

[2] *University of Johannesburg*

Corresponding Author: ncubeanele4@gmail.com

The literature on the computation of black hole quasinormal modes (QNMs) is replete with the adoption of various approximation methods to solve the "quasi-Sturm Liouville" type problems governing the damped oscillations that dominate the ringdown phase of the time-evolving signal produced by perturbed black holes. Among the newest techniques is the physics-informed neural network (PINN) algorithm, a machine learning-based, general-purpose differential equation solver that has recently been implemented successfully to compute the QNMs of Kerr black holes perturbed by gravitational fields (of spin-weight, $s = -2$). Considering the recent work showing the significance of QNM overtones early in the gravitational wave signal (just following the peak strain amplitude), we utilise PINNs to compute QNM frequencies associated with overtone numbers $n > 0$ and the dominant $\ell = m = 2$ harmonic. The performance of PINNs is then compared with extant approximation methods for QNM computation.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Theoretical and Computational Physics / 47

Quasinormal excitation factors in the eikonal regime

Authors: Anna Chrysostomou[1]; Alan Cornell[2]

[1] *University of Johannesburg*

[2] *University of Johannesburg*

Corresponding Author: achrysostomou@uj.ac.za

In the wake of a perturbation, a black hole will radiate gravitational waves (GWs). After an initial response to the external stimulus, the GW spectrum of the perturbed black hole is dominated by a discrete set of complex quasinormal frequencies (QNFs) whose values depend exclusively on the characteristic black hole properties of mass, spin, and charge. For this reason, quasinormal modes (QNMs) have become ubiquitous in black hole studies; they have come to play a prominent role in the description of astrophysical black hole merger events, tests of numerical relativity, and a possible link between gravitation and quantum mechanics. With the advent of GW astronomy, we now have the opportunity to test theoretical and numerical QNM models against GW data. In this talk, I shall discuss an asymptotic expansion method that exploits a geometrical interpretation of QNMs to compute the QNFs of spherically-symmetric black hole space-times. This method can be extended to the computation of QNM wavefunctions, and the "quasinormal mode excitation factor" (QNEF): a quantitative measure of the detectability of the QNMs that is intrinsic to the black hole source. I shall describe how we refine and extend this method, and provide examples of how QNEFs manifest in different space-times.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics for Development, Education and Outreach / 48

A review of the South African Institute of Physics (SAIP) roles in Physics for development, Education, and Outreach: Hindsight, foresight, and opportunities for South Africa through the hub-and-spoke model

Author: Brian Masara[1]

Co-authors: Deena Naidoo [2]; Makaiko Chithambo [3]; Rudolph Erasmus [4]

[1] *SAIP*

[2] *School of Physics, University of the Witwatersrand*

[3] *Rhodes University*

[4] *University of the Witwatersrand*

Corresponding Authors: m.chithambo@ru.ac.za, brian.masara@saip.org.za

The SAIP plays a pivotal role creating a platform for physicists to network, collaborate, support one another, communicate their subject, influence science and technology policies, promote the study and applications of physics, monitor the quality standards of physics training, and foster the development of physics in South Africa. This presentation highlights how the SAIP has delivered on these critical roles, reviews opportunities for improvement, and how the physics community can be involved. SAIP education, outreach and women in physics activities are implemented through the hub-and-spoke model, providing an opportunity for broad-based participation and involvement.

SAIP has over the years engaged with physics development, initiatives include hosting the Word Conference on Physics and Sustainable Development in 2005, the review on shaping the future of physics in South Africa, the formation of NITheP, SA-CERN research, SANReN, entrepreneurship for physics, and physics in industry day, among others. However, reviewing publications on WOS authored by South Africans about Physics and sustainable development, one finds less than 5 articles showing a dire need for the physics community to be involved in matters related to physics and sustainable development. Under outreach and public understanding of physics, SAIP has developed resources ranging from careers booklets to videos such as the Physics in our Everyday Life series, participates in the National Science Week, Science Festivals, and radio campaigns. Programmes such as "Physics in my Village Competition" and the South African Physics Olympiad (SAPhO) have facilitated naturing young talent into physics. Through the Women in Physics in South Africa (WiPiSA) programme, projects such as the Women in Physics lunches, and Women in Physics August month celebrations are now a permanent feature. Over the last three years, the average impact from these outreach programmes was over 2 million people per annum. In 2008, Physics HoDs raised concerns about the weak background of new first-year students, the SAIP commissioned a review and produced a benchmark statement on physics training that was adopted in 2019. During the period, 2020-2023, 18 teacher workshops were held where 1017 teachers participated, and 146 facilitators were trained. Given the shortage of physics laboratory facilities in schools, training on virtual physics experiments was introduced in 2022. Preliminary evaluations showed that teachers' confidence in facilitating the Physical Science Virtual experiments improved by 32.96 %, i.e., from 51.80 % to 84.76 %. The Essential Skills for Matric resources were introduced in 2020 and over 30 000 booklets and 2000 USBS were distributed reaching over 330 schools and 11537 learners in 7 provinces. An additional 2952 individuals accessed the materials online.

A monitoring and evaluation report based on qualitative and quantitative programme evaluation results from the teacher development and outreach programmes will be discussed. Preliminary analysis indicate that the education programme is making a positive impact. Quantitative feedback

indicated that teachers' competence improved by between 10% and 40%, however, rigorous impact analysis is required, and this presents a research opportunity. From a strategic point, the SAIP is probing the effectiveness of these interventions, how they can be improved, how can more physicists be involved, can we track the beneficiaries, etc.? These are research questions for physicists to help SAIP answer.

Key Words: Physics education, physics outreach, physics for development, women in physics, hub-spoke model, monitoring and evaluation, impact assessment

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Consent on use of personal information: Abstract Submission:

Yes, I ACCEPT

Theoretical and Computational Physics / **49**

Topological Edge States in 2D Su–Schrieffer–Heeger Models

Authors: Chani van Niekerk[1]; Robert Warmbier[2]

[1] *University of Johannesburg*

[2] *University of the Witwatersrand*

Corresponding Author: chanivanniekerk@gmail.com

Topological behaviour in optical systems and low dimensional materials has been studied widely over the last several years. In materials topological states are of special interest as they promise to exhibit protected conducting surface states in otherwise insulating systems. The protection here refers to any symmetry-preserving perturbation to the system.
For rectangular lattices the 2D Su–Schrieffer–Heeger (SSH) model is a common choice for materials with particle-hole and chiral symmetries. In two-dimensional materials specifically topologically protected corner and edge states can occur. Edge states are usually identified with some weak notion of topology, but they are more interesting for applications needing to drive some surface current.
We present here the standard SSH model as well as a new extended SSH model including second-nearest-neighbour (SNN) interaction. For these models the characteristic topological phases are presented. The standard SSH model presents phases with corner as well as edge states. The zero energy corner state is suppressed in semi-periodic configurations allowing for the edge state to be the lowest energy state. We further show the influence of symmetry-breaking SNN interactions. These leave the edge states virtually unchanged, but shift and deform the bulk bands, allowing us the engineer a desired band structure and topological state.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Consent on use of personal information: Abstract Submission:

Photonics / **50**

Quantum random number generation using an on-chip linear plasmonic beamsplitter

Author: Conrad Strydom[1]

Co-author: Mark Tame [1]

[1] *Stellenbosch University*

Corresponding Author: conradstryd@gmail.com

True random numbers are ubiquitous in cryptography, simulation and many other information processing tasks. Here we experimentally demonstrate quantum random number generation with an on-chip linear plasmonic beamsplitter. The beamsplitter has a footprint of 2μm x 10μm and is more compact than a previous demonstration, with a reduction in size by a factor of 2, thereby reducing the impact of loss. At the input grating of the beamsplitter, free-space single photons are converted into single surface plasmon polaritons which propagate along one of two gold stripe waveguides to one of two output gratings where they are converted back into photons. The value of each random bit is determined by the output at which each photon is detected. In our experiment, we achieved a random number generation rate of 2.86 Mbits/s, despite the presence of loss. By applying randomness extraction in the form of a deterministic shuffle followed by the recursive von Neumann algorithm to the generated bits, we obtained a sample of bits which passed the ENT and NIST Statistical Test Suites.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Astrophysics & Space Science / 51

ULXs as progenitors of merging compact binary systems

Authors: Lutendo Nyadzani[1]; Soebur Razzaque[2]

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Using Ultra-Luminous X-ray (ULX) sources as progenitors of compact binary systems, we estimate the coalescence rate of compact binary systems. ULXs are extra-galactic X-ray sources with apparent luminosity > 10^{39} erg/s. They are thought to be accreting NS or BH. The mechanism of how these systems reach such high luminosity is still unknown. 10^{39} erg/s is above the Edington accretion limit for a 10M_{\odot} BH. There are a few explanations for such high luminosities: (1) NS/BH accreting at super-Eddington accretion rate, (2) highly beamed emission, and (3) emission from an intermediate-mass black hole with a mass of 100M_{\odot} to 10^5M_{\odot} at sub-Eddington accretion. Observation of some ULX systems suggests NSs accreting with beamed emission with massive companions. Eventually, some of these companion stars will become compact objects, forming compact binary systems which are potential progenitors of gravitational waves and short GRBs. Assuming all merging compact binary systems undergo a ULX phase, we simulate a population of binary stars and follow their evolutionary history. We compute the merger rate from the compact binaries that went through a ULX phase.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / **53**

The use of Machine learning to improve quality control in electronics for CERN.

Author: Khathutshelo Phadagi[1]

Co-authors: Bruce Mellado [1]; Edward Nkadimeng [1]; Ryan Mckenzie [2]; Tristan Jade Wilkinson [1]

[1] *University of the Witwatersrand*

[2] *University Of the Witwatersrand*

Corresponding Author: khathutshelo.tony.phadagi@cern.ch

This paper demonstrates how using deep neural networks can improve quality control of Low Voltage Power Supply (LVPS) Boards. Deep Neural Networks (DNNs) as a machine learning algorithm is used to analyze complex data from the LVPS Boards. The first initial testing done on the boards determines their reliability and performance. A total of eleven tests with a binary metric of PASS/FAIL make up the initial test station. The measurements are stored in a database. The multi-dimensional data that Is labelled is explored and then anlayzed by a DNN algorithm. The DNN model classifies the data, and produce significant insights with predictions about the quality of the LVPS boards. These forecasts will help the European Organization for Nuclear Research (CERN) with Quality Control of the Toroidal Large Hadron Collider Apparatus (ATLAS) Tile Calorimeter (TileCal) Phase-II LVPS Brick upgrading Bricks. Preproduction and production has been approved for this year, the LVPS boards will produce more data than prior research used. I will explain the importance of the LVPS bricks and how Machine Learning is improving the quality control of electronics.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Applied Physics / **54**

Fast neutron transmission spectroscopy for the non-destructive analysis of concrete

Author: Naledi Segale[1]

Co-authors: Tanya Hutton [1]; Sizwe Mhlongo [1]; Andy Buffler [1]

[1] *University of Cape Town*

Corresponding Author: sglnxx001@myuct.ac.za

Concrete in nuclear facilities is primarily used to provide structural support, radiation shielding, containment and protection against internal and external hazards. Over its lifetime, the concrete will

be exposed to unfavourable conditions such as corrosion, radiation, extremely varying temperatures and cyclic loadings. Exposure to these conditions leads to deterioration and loss of moisture thus compromising the shielding and structural integrity of the concrete [1,2]. This becomes relevant when considering the long-term operation of nuclear facilities. The Koeberg nuclear power plant (NPP) is nearing the end of its planned lifetime, and Eskom, overseen by the National Nuclear Regulator (NNR), is aiming to extend the life of the NPP by an additional 20 years [3]. Non-destructive measurements of the water content of these existing concrete structures are crucial to the process, both in terms of radiation shielding properties and the accuracy of Monte Carlo based radiation transport simulations [4].
In fast neutron transmission spectroscopy, the sample of interest is irradiated with a well-characterised beam of neutrons, and the transmitted neutron spectrum can be used to infer the elemental composition through a deconvolution technique [5]. In this work, we present an experimental and simulated verification of the technique using sand, a primary constituent of any concrete. Measurements were made at the n-lab at UCT [6] using a collimated beam of neutrons produced by an americium-beryllium (AmBe) neutron source, and samples of sand and its constituents CaCO3 and SiO¬2. Transmitted neutron energy spectra were measured using an EJ-301 organic liquid scintillator coupled with spectrum unfolding techniques, and subsequently used to determine the energy dependent effective removal cross section for each sample. A comparison was made with the removal cross sections obtained from simulations with FLUKA to validate the use of simulated data where physical measurements were impractical. The calculated ratios of CaCO3 and SiO2 in sand were verified against those obtained by x-ray fluorescence.

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[2] Naus, D.J. et al., Nuclear power plant concrete structures – aging consideration, Challenges of Concrete Construction: Volume 6, Concrete for Extreme Conditions, pp. 747–764 (2002).
[3] World Nuclear News, Review of Koeberg extension plans completed by IAEA Team (2022).
[4] Petit, M., Concrete modeling for neutron transport and associated sensitivity stud- ies performed at the AMANDE-MIRCOM facility. Nucl. Sci. Eng., 195:8, 846 (2021)
[5] Hutton, T., Buffler, A. and Alexander, M. Elemental analysis of concrete via fast neutron transmission and scattering spectrometry, EPJ Web Conf., 261, 03003 (2022).
[6] Hutton, T. and Buffler, A., A new D-T neutron facility at UCT, Proc. SAIP2017, pp 324-330 (2018).

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Applied Physics / 55

EFFECT OF NANO-SCALED METAL OXIDES ON THE CARBON-NITROGEN RATIO OF COW DUNG FOR SUSTAINABLE BIOGAS PRODUCTION

Authors: Takalani Nethavhanani[1]; Eric Maluta[2]; Vhutshilo Nekhubvi[2]

[1] *University of the Western Cape*

[2] *University of Venda*

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Over the past decade, South Africa has experienced massive scheduled power outages due to the inadequate generation capacity of coal-fired power plants. This ongoing crisis is likely to continue if researchers do not look for alternative methods to solve South Africa's poor energy supply. One alternative solution that could prevent South Africa from this crisis is using clean energy such as

solar, wind, biomass, etc. Studies have shown that methane produced by anaerobic digestion offers enormous potential as a renewable energy source. Anaerobic digestion (AD) technology is one of the most popular renewable energy technologies. During AD, bacteria break down organic matter - such as animal manure, solid wastewater, and food waste -into biogas without oxygen. Biogas consists primarily of methane (CH4) and carbon dioxide (CO2), with minimal water vapour and other gases. Although AD technology is widely used, its low biodegradability and biogas production limits its commercial application. Hence, the use of nanoparticles (NPs) as additives has been extensively investigated and shown to significantly improve AD performance and biogas production. The NPs mostly used as additives in the AD process are zero-valent metallic NPs, metal oxide NPs, carbon-based nanomaterials, and multi-compound NPs. However, recent studies have found that metal oxide NPs are more suitable for enhancing biogas and CH4 production. This study, therefore, investigates the effect of metal oxide nanoparticles on anaerobic digestion with the aim of experimenting using local organic materials for biogas production. The potential nano-additives to be explored are calcium oxide (CaO), iron oxide (Fe2O3/Fe3O4), potassium oxide (K2O), magnesium oxide (MgO), manganese oxide (MnO2), and phosphorus pentoxide (P2O5), and titanium oxide (TiO2).

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Consent on use of personal information: Abstract Submission:

Poster Session 1 / **56**

Binding nature of fibrin molecules on to Au92 and Ag92 nanoparticles

Authors: Malesela Walter Makgoba[1]; Thuto Mosuang[2]; Mokete Mahladisa[2]; Malili Matshaba[2]; Rapela Maphanga[3]; Lucky Sikhwivhilu[4]; Teboho Mokhena[4]

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[2] *University of Limpopo*

[3] *CSIR*

[4] *Mintek*

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Density functional theory, and molecular dynamics simulations were used to study the nature of binding on Au- and Ag-nanoparticles and 1, 2, and 3-fibrin molecules. In the process, the negative adsorption energies acquired suggest that the fibrin molecules + Au-/Ag-nanoparticles reaction process is exothermic and energetically stable. Moreover, radial distribution functions and radius of gyration were utilised to explore the binding distance between the fibrin molecules functional groups atoms and Au-/Ag-nanoparticles surface atoms. To probe the mobility of the atoms in the fibrin-nanoparticle complexes, the mean square displacements graphs were plotted. Such plots together with the extracted diffusion constants suggest that H, C, N and O from the fibrin molecules functional groups, may diffuse easily into Au- and Ag-nanoparticles. Qualitatively, the H, C, N, and C atoms diffuse more readily in the Ag-nanoparticles compared to Au-nanoparticles.

Apply to be considered for a student ; award (Yes / No)?:

YES

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Astrophysics & Space Science / **57**

Investigating the Role of Turbulence in Solar Energetic Particle Transport

Author: Jaclyn Stevens[1]

Co-author: Du Toit Strauss [2]

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Understanding the mechanisms behind Solar Energetic Particle (SEP) transport in the inner heliosphere aids in the effort to develop accurate and predictive space weather models.
Modelling several sets of observations over different events by the Solar Orbiter, WIND, GOES, and SOHO spacecraft, at a distance between 0.3 - 1.0 AU, provides transport parameters that cannot be measured or observed.
Of these parameters, the results for the mean-free-path of the particle are compared to theoretical estimates.
Combining theory, observation, and analytical results provides more insight into future predictive models of SEP intensity.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Astrophysics & Space Science / **58**

Possible origins of > 10 TeV photons detected from the burst of all time (BOAT) GRB 221009A

Author: Soebur Razzaque[1]

[1] *University of Johannesburg*

Corresponding Author: srazzaque@uj.ac.za

Gamma-Ray Burst (GRB) 221009A was once in a century event detected from radio to very high-energy (VHE) gamma rays. It was the first time that > 10 TeV gamma rays were detected from a GRB. Even though GRB 221009A was a relatively nearby event at redshift 0.15, detection of a 18 TeV photon by the LHAASO detector and of a 251 TeV photon by the Carpet-2 detector challenge conventional radiation mechanisms of a GRB and/or propagation of VHE gamma rays in the cosmic radiation backgrounds. In particular, gamma-ray flux at 18 TeV is expected to be attenuated by a factor $\sim 4.5\times10^{-5}$ and more severely at 251 TeV due to $\gamma\gamma \to e^{\pm}$ pair production by interacting with the photons of the extragalactic background light (EBL). In this presentation, I will discuss possible explanation of the detection of 18 TeV photon due to ultrahigh-energy cosmic rays originating from GRB 221009A and interacting while propagating along the line-of-sight [1], and the detection of 251 TeV photon due to violation of Lorentz invariance [2].

[1] S. Das and S. Razzaque, "Ultrahigh-energy cosmic-ray signature in GRB 221009A," Astron. Astrophys. **670,** L12 (2023) [arXiv:2210.13349 [astro-ph.HE]].

[2] J. D. Finke and S. Razzaque, "Possible Evidence for Lorentz Invariance Violation in Gamma-Ray Burst 221009A," Astrophys. J. Lett. **942**, no.1, L21 (2023) [arXiv:2210.11261 [astro-ph.HE]].

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Nuclear, Particle and Radiation Physics / **59**

Evaluation of the significance of a scalar candidate at 95 GeV at the LHC

Author: Thabo Pilusa[None]

Co-authors: Bruce Mellado [1]; Salah-eddine Dahbi [2]

[1] *University of the Witwatersrand*

[2] *University of Wits*

Corresponding Author: pilusajustin@gmail.com

Motivated by an excess around 95 GeV in the LEP data, we evaluate several excesses around that mass that have emerged in recent years at the Large Hadron Collider (LHC). Results from the CMS and ATLAS collaborations have shown that there is a scalar at around that mass, we combine the results from both collaborations for when the scalar decays into $\gamma\gamma$, $\tau\tau$, and WW to analyze the significance. The potential connection of this scalar candidate with the multi-lepton anomalies at the LHC is discussed.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Nuclear, Particle and Radiation Physics / **60**

A search for tWZ production at $\sqrt{s}$=13TeV with the ATLAS detector

Authors: Alexander Veltman[1]; JAMES KEAVENEY[1]

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Corresponding Author: vltale001@myuct.ac.za

The production of a single top quark in association with a W boson and a Z boson (tWZ) is a rare Standard Model process which has never before been measured. This process will be a useful input into global Standard Model Effective Field Theory (SMEFT) fits due to its sensitivity to top-electroweak SMEFT coefficients in regions of high W boson and Z boson transverse momenta. It is

also a relevant background in other top quark related measurements such as the $t\bar{t}Z$ cross section measurement. A search has been performed for tWZ production using 140fb^{-1} of proton-proton collision data at a centre of mass energy of 13 TeV. The search targets the trilepton and tetralepton final states. Regions are defined using physics object multiplicities and graph neural networks are employed to perform signal-background discrimination. The signal strength of tWZ production μ_{tWZ} is extracted using a profile likelihood fit with a full systematic model describing experimental and modelling uncertainties. Preliminary blinded measurements of μ_{tWZ} are shown for each channel using an Asimov data set. A combined signal extraction across both channels will also be presented. The measurements of μ_{tWZ} shown will include their associated expected significance and expected upper limits. Estimations of the measurements of μ_{tWZ} for higher luminosity data sets are investigated.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Astrophysics & Space Science / **61**

Kepler and Gaia DR2 views of open cluster NGC 6819

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[1] *University of Zululand*

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In this work we derive the distance modulus from Gaia parallaxes for Kepler Input Catalogue (KIC) stars located within 10 arcmin in the field of NGC 6819. The mean distance modulus is used to determine probable new KIC members of NGC 6819 cluster. We find 7 probable KIC new astrometric distance members which have been previously overlooked in the literature as revealed by Gaia Data Release 2 (DR2). Of these, one is a solar-like star (SOLR), one γDor star (GDOR), 2 rotational variables, 1 eclipsing binary and 2 unknown types. There is no significant difference in the mean distance modulus when probable new astrometric members are included in deriving the mean distance modulus.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

NA

Astrophysics & Space Science / **62**

Solar energetic particle transport between Earth and Mars

Author: Aimée Dumont[1]

Co-author: Du Toit Strauss [2]

[1] *North-West university*

[2] *Centre for Space Research, North-West University*

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Observing and modelling solar energetic particles (SEPs) aids to establish an early warning system to prevent any hazardous impact on humans and technology in space. Using the electron intensity observations from the MAVEN and WIND spacecraft, one-dimensional SEP transport is simulated during MAVEN's voyage along the Parker-Hohmann orbit from Earth to Mars. The soft X-ray data from GOES was used to approximate the injections of the SEPs in the model. The data is then used to determine if the SEPs followed the same trajectory along the Parker-heliospheric magnetic field. The understanding of SEP behaviour along the Parker-Hohmann orbit will be necessary for future crewed missions to Mars.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

Hons

Physics of Condensed Matter and Materials Track 2 / 63

Computational studies of pressure dependence on Monazite-(Ce)

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Co-authors: Ramogohlo Diale [2]; Reneir Koen [3]; Phuti Ngoepe [1]; Hasani Chauke [1]

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Monazite-(Ce) is an orthophosphate mineral of the monazite group with the formula A[PO4], where A represents Ce and other light rare earth elements (LREE) in place of Ce. Studying the structural stability of monazite-(Ce) is of vital importance in the storage of radioactive waste application. A first-principle calculation based on density functional theory was used to study the structural, mechanical, and vibrational properties of Monazite-Ce under different pressure range from 10-50 GPa. The calculated structural parameters of monazite systems at zero pressure and temperature agree with the experimental data within 5 %. The Modulus (Bulk, Shear, Young's), and anisotropy increase with an increase in pressure. Furthermore, Pugh (B/G) and Poisson ratio show that monazite system is ductile and the ductility can be improved with an increase in pressure. The vibrational instability of the CePO4 system is observed which is caused by the soft mode detected from the phonon dispersion curve. However, the system becomes vibrationally stable when the pressure is increased. The insights gained from high-pressure studies are of interest for the applications of monazite.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / **64**

Computer simulation of Silver (Ag) and Nickel (Ni) Nanomaterials

Authors: Malili Matshaba[1]; Natasha Makhathini[None]; Mokete Mahladisa[1]; Thuto Mosuang[1]

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Silver and nickel nanomaterials have attract increasing attention for the wide range of applications. Most of their applications are for industrial purposes, high electrical conductivity, automotive catalytic converters, health care, etc. Their applications can be maximized by studying their structural and electronic properties. In this work we utilize molecular dynamics simulation to investigate their properties and energies in relation to different temperature. We also investigate their radial distribution functions for both systems. All calculations will be performed using Sutton-Chen potentials and a computer code called DL Poly code.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 2 / **65**

Molecular dynamics studies of the transfer of protons in multi-walled carbon nanotube poly(2,5)benzimidazole composites

Authors: Salomon van Niekerk[1]; Lynndle Square[2]

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In Low Earth Orbit (LEO), some dangers spacecraft electronics are subjected to are high energy protons [1]. Their energies range from a few MeV to GeV [2]. The current shielding employed by spacecraft (consisting mainly of satellites) is insufficient in protecting internal electronics [3]. In the past, and still, an extensively researched avenue is to employ polymers and composites as a radiation shielding mechanism [4]. This is due to their desirable lightweight and excellent mechanical properties [4]. One such polymer meeting this criterion is Poly(2,5)benzimidazole (ABPBI) [5] and ABPBI with multi-walled carbon nanotube (MWCNT) enhancement. Its interactions with energetic protons were investigated using molecular dynamics (MD) [6]. The mean square displacement (MSD) and radial distribution function (RDF) [7] reported in this work aid in seeing how these interactions change due to different weight percentages (1%, 3%, and 5% load of MWCNT). A Perl script was implemented to quantify and monitor variations in the paths available in the samples for proton hopping. These methods help indicate the most likely path the energetic proton moved through [7]. This investigation considers the efficacy of using ABPBI, and its composites, as a proton shielding material for LEO spacecraft applications and further considers changes due to adding carbon nanotubes.

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Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Consent on use of personal information: Abstract Submission:

Astrophysics & Space Science / 66

Modelling galactic cosmic ray drifts in the presence of a Fisk-type heliospheric magnetic field

Authors: Jonathan Stephanus Troskie[1]; Nicholas Eugene Engelbrecht[1]; Petrus Johannes Steyn[1]

[1] *NWU Centre for Space Research*

Corresponding Author: jst99960@gmail.com

Drift effects due to gradients and curvature in the heliospheric magnetic field (HMF) have long been known to affect cosmic ray (CR) modulation. Thus far, only drift effects due to the geometry of the HMF proposed by Parker (1958) have been studied. However, several other HMF models exist, including the model proposed by Fisk (1996), which, notably, has a latitudinal component. The Fisk-Parker hybrid HMF proposed by Burger & Hitge (2004) assumes that the HMF is Parkerian at the poles and in the ecliptic plane, and Fisk-like at mid-latitudes. In this presentation, the effects of the Fisk-Parker hybrid HMF on CR drifts are discussed; these results show, for the first time, that a Fisk-type HMF results in a CR drift velocity profile which differs significantly from what has first been described for the Parker HMF by Jokipii & Thomas (1981). Furthermore, different approaches to modelling drift due to the heliospheric current sheet are investigated; these include the models proposed by Burger (2012) and Engelbrecht et al. (2019).

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics for Development, Education and Outreach / 67

DEVELOPING GRADE 12 LEARNERS CONCEPTUAL UNDERSTANDING OF CHEMICAL EQUILIBRIUM USING PROBLEM-BASED LEARNING

Authors: Prudence Modjadji Mamabolo[1]; Phala Masoga[1]

[1] *University of Limpopo*

Corresponding Author: prudence449@gmail.com

This study aimed to develop learners' conceptual understanding of chemical equilibrium, using problem-based learning. The study used a qualitative research approach with ethnography as a design. Data was gathered from a rural school in Dimamo circuit of the Capricorn district in the Limpopo Province. The school had 24 learners in the grade 12 Physical Science classroom. Participatory observation, learner activities, and interviews were used in the initially in the study to identify learners' lack of skills and their learning difficulties. Problem-based learning was then applied continuously and repeatedly during the teaching and learning activities. It was shown that problem-based learning helped develop learners' conceptual understanding of chemical equilibrium. Thematic analysis was used to categorise and present data-related themes. Descriptive statistics was used to analyse the data generated during the intervention. The study discovered that learners lacked the mathematical computational skills and procedural fluency required for competence in this subject. Furthermore, the ability to apply Le Chatelier's principle to problems and identifying factors that affect kc and the equilibrium constant was also a hindrance to effective learning. The post-test revealed that learners' conceptual understanding improved following problem-based learning instruction. Moreover, the study also discovered that integrating new concepts with mathematical calculations, and theoretical justification can help learners improve their conceptual understanding. In conclusion, the concept requires the use of problem-based learning to further motivate learners and help them grasp the content and learn with understanding.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

Honours

Poster Session 2 / 68

RESISTIVE SWITCHING IN AG/CS+PVP+CDTE/CDSE/ITO-PET DEVICE FOR APPLICATION IN ECO-FRIENDLY MEMORY DEVICE

Authors: Khanya Giba[1]; Zolile Wiseman Dlamini[2]; Sreedevi Vallabhapurapu[1]; Vijaya Srinivasu Vallabhapurapu[3]; Olamide Abiodan Daramola[4]

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[2] *Department of Maths, Science and Technology, Central University of Technology*

[3] *Physics Department, University of South Africa*

[4] *Department of Chemical and Physical Science, Walter Sisulu University*

Corresponding Author: khanyagiba@gmail.com

Electronic devices that are made primarily of organic materials are significant for reducing electronic waste. The resistive switching properties of a chitosan/polyvinylpyrrolidone (PVP) polymer blend dispersed with CdTe/CdSe core-shell quantum dots are investigated. Both chitosan and

polyvinylpyrrolidone (PVP) are non-hazardous to the environment. This composite was employed in the active layer of a resistive switching memory (ReRAM), which employs silver and indium doped tin oxide electrodes. The device's electrical characterisation indicated that it had asymmetric "S-type" memory behavior with a I_{ON}/I_{OFF} ratio of ≥ 10 and a very low (0.2 V) working voltage, making it suitable for low power consumption device applications. Furthermore, the presence of CdTe/CdSe in the composite was thought to enhance the Schottky barrier height of the interface between the electrodes and the active layer, resulting in the creation of conductive filaments due to silver electrode diffusion into the active layer. Overall, our findings suggest that by including CdTe/CdSe QDs, the memory and switching behavior of the chitosan/PVP blend-based resistive switching memory may be utilized.

Apply to be considered for a student ; award (Yes / No)?:

YES

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / **69**

Structural and Vibrational Studies of TbMn2O5 Powder

Author: Geoffrey Mwendwa[1]

Co-authors: Adam Shnier [2]; Aderemi Haruna [2]; Daniel Wamwangi [1]; Dave Billing [2]; Hugo Dil [3]; Kenneth Ozoemena [2]; Lesias Kotane [4]; Milan Radović [5]; Morgan Madhuku [6]; Rudolph Erasmus [1]

[1] *School of Physics, Material Physics Research Institute, University of the Witwatersrand, Johannesburg, South Africa*

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[3] *Institut de Physique, École Polytechnique Fédérale de Lausanne, Switzerland*

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Multiferroic rare-earth composite oxides with a perovskite-like structure such as terbium manganites hold a wide range of correlated properties for next-generational devices characterized by high efficiency, low energy dissipation, and high storage density among other high-end capabilities. Some of the envisaged applications include solid-state refrigeration, 4-state memory storage, ferroelectric photovoltaics, and spintronic devices.

In magnetoelectrics, ferroic orders (ferromagnetism and ferroelectricity) occur in the same phase by the virtue of symmetry breaking, which in this case is manifested in the form of crystal structure distortion. Motivated by the fundamental question of the structure-function relationship in these materials, we have synthesized TbMn2O5 powders (substrate-free nanostructures) by a sol-gel-based method.

The composition fidelity of the sample was probed and validated by SEM-EDX. Rietveld refinement shows that the as-synthesized sample has three phases: TbMn2O5 (89%), TbMnO3 (6%), and Mn3O4 (5% by volume). Except for the mode at 105 cm-1, all Raman modes of Ag, B1g, B2g, and B3g symmetry expected for the Pbam structure have been observed.

Keywords: Multiferroics, ferroic orders, magnetoelectric effect

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 1 / 70

Effect of Gd3+ moles on the structure, morphology and luminescence properties of BaAl2O4:x% Gd3+ (0 ≤ x ≤ 1) nanomaterial prepared using a sol-gel method.

Author: Livhuhani Malinga[1]

Co-authors: Rebecca Mhlongo [2]; Thabang Melato [1]; Vusani Maphiri [2]; Clinton Dlamini [1]

[1] *Vaal University of Technology*

[2] *Sefako Makgatho Health Sciences University*

Corresponding Author: rebsmhlongo@gmail.com

In this study BaAl2O4:x%Gd3+ (0≤ x≤ 1) nanomaterial were prepared using sol-gel mathod. X-ray diffraction (XRD) data revealed that all samples consisted of a single phase of cubic BaAl2O4 structure with no impurities. Fourier Transformation Infrared spectroscopy (FTIR) revealed four absorption bands at 843, 1016, 1416, and 3434 cm-1. The presence of Ba, Al, O and Gd were confirmed by the energy dispersive Xray spectroscopy (EDS). Scanning electron microscope (SEM) revealed that the morphology of the prepared samples highly depends on the Gd3+ concentration. Transmission electron microscopy (TEM) results revealed the tubular rods and nano-nature of the crystallite sizes. Photoluminescence (PL) spectroscopy results revealed three emission peaks located at 414 nm, 436 nm, -and 748 nm . All the emissions are from the host, all this emissions are attributed to arise from the intrinsic defects within the host material such as oxygen. The results revealed the Gd3+ optimum intensity at 0.6% Gd3+. This suggests that increasing the concentration of Gd3+ in the host influences the luminescence of the nano-powders. The International Commission on Illumination (CIE) colour showed that the violet emission colour of the prepared samples depends on the excitation wavelength and Gd3+ concentration.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 2 / 71

Investigation of surface stability and interaction of thionocarbamate collectors on pentlandite (Fe5Ni4S8) mineral

Authors: Nontobeko Zavala[1]; peace prince mkhonto[1]; Phuti Ngoepe[1]

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Abstract
Pentlandite is the primary source of nickel as well as a major carrier of platinum group elements

(PGEs). Nickel mining is popular in many nations, contributing to a variety of industrial applications such as stainless steel, coinage, and rechargeable batteries, which contribute to the ever-increasing demand for nickel, which is expected to run out by 2030. The flotation in pentlandite and nickel ore has always been performed using various collectors such xanthates, dithiophosphate and dithiocarbamate. Density functional theory computational method was used to determine the most stable surface and the preferred cleavage of Fe5Ni4S8. The bulk structure was determined by cluster expansion. The (100), (001), (110), (101), (111), (211) and (112) surface were cleaved from the relaxed bulk structure and their surface energies were computed. It was found that the (001) surface gave the lowest positive surface energy and therefore the most stable surface. Moreover, the reconstruction of the (001) surface indicated that the reconstructed surface was more stable compared to the un-reconstructed surfaces. The adsorption of O-isopropyl-N-diethyl-thionocarbamate (IPDETC) on the reconstructed Fe5Ni4S8 (001) surface was performed on Fe and Ni sites and showed strong adsorption. This suggested that IPDETC collector may be used in the flotation of pentlandite mineral.
KEYWORDS
Computational modelling, Fe5Ni4S8 pentlandite, Surface reconstruction, Surface energies, IPDETC, Adsorption energies

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / 72

Reactive molecular dynamics simulations of the atomic oxygen impact on Poly(2,5-benzimidazole)

Authors: Ernst Ellis[1]; Lynndle Square[2]

[1] *North-West University*

[2] *North West University*

Corresponding Author: impie12@hotmail.com

The development of radiation shielding for spacecraft found in low Earth orbit (LEO) has been an ongoing campaign since 2001 [1, 2]. In the LEO range, various threats cause extensive degradation of spacecraft materials. Considering organic materials such as polymers have one threat that significantly affects them: atomic oxygen (AO). Atomic oxygen is formed via photo-disassociation of diatomic oxygen caused by solar radiation [3] with a flux of $\sim 10^{14} AO/cm\ s$ at energies of ˜5eV [4]. AO is the most abundant species found in the LEO environment and causes oxidative erosion of organic material. Testing the erosive nature of AO on a polymer proves difficult when considering the experimental apparatus required to replicate the AO impact on the material [4]. This difficulty is the availability of apparatus that can have AO as the bombardment species while performing the bombardment experiment at the required energy. In South Africa, very few nuclear accelerators have AO as the bombardment species, but these have energy constraints. A model is created for this investigation to perform AO bombardment on the poly(2,5-benzimidazole) (ABPBI) material and composite variations using reactive molecular dynamics (MD). The results from the MD simulations include mass loss, AO penetration depths, and temperature evolution with regards to AO impact on the material. In previous work, the authors performed AO bombardment on the polymer and its composite at the iThemba labs Gauteng. The intention of this work is to, through the reactive MD, compare changes to the samples as a result of varying energies.

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Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

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Nuclear, Particle and Radiation Physics / **73**

Statistical Properties of Xe-133 from Inverse Kinematics Reactions using Ratio Method.

Authors: Teffo Seakamela[1]; Bonginkosi Kheswa[2]; Mathis Wiedeking[3]; Simon Connell[4]

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[2] *University of Johannesburg*

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Corresponding Author: teffoseakamela@gmail.com

Abstract. A substantial number of experimental studies over the years have shown that many light-to-medium-sized and some rare-earth nuclei exhibit a Low-Energy Enhancement (LEE) in the Gamma Strength Function (GSF) [1,2,3,4 and references therein]. Within the Hauser-Feshbach formalism, the GSF and the Nuclear Level Density (NLD) play crucial roles in the estimates of nuclear reaction rates. It has been demonstrated that the presence of this LEE can significantly speed up astrophysical r-process reaction rates [5] for neutron-rich nuclei. This should be further researched because it would have a big impact on models of nucleosynthesis. Due to the difficulty in creating adequate targets, experimental data on the LEE for noble gas isotopes like 133Xe are also non-existent. At the iThemba LABS, 132Xe (d,p) reactions in inverse kinematics were carried out with beam energy of 530 MeV in order to look for the LEE in the 133Xe nucleus. In conjunction with a silicon particle telescope that was used to measure the charged particles from the reactions, the AFRODITE and ALBA arrays were utilized to measure the gamma-rays. Eight high resolution germanium detectors, six large and six small volume LaBr3(Ce), and two S2 silicon strip detectors made up the array at the time of the studies. Particle-□-□ events event extraction and the Ratio Method are being utilized to determine the GSF of 133Xe.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics of Condensed Matter and Materials Track 1 / 74

Evolution of magnetic ground state in $A\mathrm{Co_2As_2}$ (A = K, Ca, Sr, Ba) system

Author: Abhishek Pandey[1]

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$A\mathrm{Co_2As_2}$ (A = K, Ca, Sr, Ba) and $\mathrm{BaMn_2}X_2$ (X = P, As, Sb, Bi) compounds that both crystallize in $\mathrm{ThCr_2Si_2}$-type tetragonal structure together present a text-book type example of how the structural parameters and electronic band structure can indirectly govern the magnetic ground state of a crystalline system. $A\mathrm{Co_2As_2}$ compounds exhibit properties that delicately depend upon the interlayer As-As distance $d_{\mathrm{As-As}}$ which regulates the oxidation state of Co-ions by controlling the extent of the interlayer As-As bonds. As a result, it controls the magnetic ground state of these materials. On the other hand, d_{X-X} does not show any significant variation within $\mathrm{BaMn_2}X_2$ compounds and because of the localized nature of d-bands, it does not affect the oxidation state of the Mn-ions as well as the magnetic ground state of these compounds. In this work, we present a comparative study on $A\mathrm{Co_2As_2}$ and $\mathrm{BaMn_2}X_2$ systems. Further, we explore the combined effect of the change of electron count as well as the increase in $d_{\mathrm{As-As}}$ introduced through the partial substitution of alkaline-earth ions in the $A\mathrm{Co_2As_2}$ system. We report on the magnetic characteristics and electron transport properties of this hole-doped system and explore the interdependency of structural parameters, charge density and many-body interactions within the material.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 1 / 75

Structural investigation of Pd/Zr/Pd/Ti/Pd multilayered system implanted with 150 keV argon ions for hydrogen storage application

Authors: Christopher Mtshali[1]; Charles Thulani Thethwayo[2]

Co-authors: Zakhele Khumalo [3]; Ceboliyazakha Ndlangamandla [2]; Puleng Biyela [2]

[1] *iThemba labs*

[2] *University of Zululand*

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A multi-layered system of titanium (Ti), zirconium (Zr), and palladium (Pd) was successfully prepared on different substrates using an electron beam evaporator (NEE-4000) for hydrogen storage applications. Ti alloy (Ti-6Al-4V) and pure commercial Ti (cp-Ti) were used as substrates to prepare stacked layers of Pd/Ti/Pd/Zr/Pd. The phase transformation was studied using X-ray diffraction (XRD) and Rutherford backscattering spectroscopy (RBS), which allowed a deep understanding of how these metals interact with each other before and after introducing hydrogen. These techniques were also used to investigate the effect of ion implantation, and the results were compared to those of as-prepared samples. XRD reveals that there was a diffusion of atoms between the layers, resulting in the formation of Ti-Pd and Zr-Pd alloys before implantation and hydrogenation; this was also

confirmed by RBS. When the samples were implanted with argon ions at different fluencies (1012, 1013, 1014, 1015, and 1016, respectively), a shift in crystal angle (2) was observed but no noticeable alteration in the crystal structures. The Pd layer was used to reduce oxidation between the Ti and Zr layers. Both prepared and implanted samples showed evidence of oxidation between the two layers, which resulted from the chamber's residual gases.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 1 / **76**

Electronic, elastic and thermoelectric properties of hexagonal CuSe phase

Authors: MOSHIBUDI RAMOSHABA[1]; Thuto Mosuang[1]

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Corresponding Author: moshibudi.ramoshaba@ul.ac.za

Density functional theory using full-potential all-electrons linearised augmented plane waves was implemented to study electronic, elastic, and thermoelectric properties of hexagonal CuSe phase. Electronic bands suggest a metallic compound of zero energy gap. Density of states further expose the electron density responsible for this metallic behaviour. Elastic properties reveal mechanical stability and the possibility of being synthesisable. The compound is less compressible with positive calculated Cauchy pressure. High values of the power factor and the Seebeck coefficient allow consideration of the phase for thermoelectric applications.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

PHD

Poster Session 2 / **77**

GAMMA COMPUTED LAMINOGRAPHY: A TROUBLESHOOTING TOOL FOR DISTILLATION COLUMNS

Author: Witness Chirume[1]

Co-authors: Caven Dzingai [2]; Joseph Dongo [3]; Peter baricholo [2]; Robin Mashingaidze [3]; Stanford mudono [3]

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Abstract
An innovative way of performing gamma column scanning was implemented in which the results are presented as a 2 dimensional density plot. Computed laminography is used for image reconstruction using experimentally obtained data to produce a 2D image from 1D projection of the column's interior. Snark14 software, which is used for 2D image reconstruction from 1D projections was used for image reconstruction. A phantom of the object to be reconstructed was designed using the Snark14 input file. A Snark14 input file based on parallel geometry for the source and detector was created according to a specific geometry. The reconstructed image of the phantom was satisfactory and this validated that the proposed geometry could be used in the physical experiment. Preliminary experiments were performed according to the specified geometry and the results are in agreement with the simulation.

Introduction
Malfunctioning in distillation columns can seriously affect plant operations and result in low yield and product quality that will lead to heavy financial losses. When a column behaves abnormally, it is necessary to investigate the distillation column and quickly rectify the problem in order to minimize losses. Gamma column scanning is the most widely used method to troubleshoot industrial equipment in the petrochemical plants. A sealed radiation source and a detector are placed on opposite side of the column and are moved simultaneously along the column and the intensity measurements are used to generate a density profile of the column. To analyse a line profile one needs to have a blend of skills and knowledge, hence the need to find a method of acquiring data and present it in the form of a 2 dimensional (2 D) image of the object being scanned, which is easier and more informative than the line profile. In order to get a 2D image some tomographic reconstruction algorithms have to be implemented. The data collection schematic of figure 1 was adopted and simulation experiments were carried out and the results showed that the proposed data collection geometry is feasible. Physical experiments were performed and the results obtained are very promising.

Methodology
A radiation source was placed on one side of the column and a detector used to measure the attenuation of the beam at different position on the opposite side of the column. The objects to be scanned were inserted into the column. Three physical scans were performed on the concrete block, mild steel pipe and a distillation column with two trays and a standard brick at the bottom. The detector was moved up from the straight through position by 15.0 cm to make an angle of 21 degrees to the horizontal. The detector was then moved in steps of 1.0 cm from 15 cm to -15 cm until 31 detector reading were taken. The source was then moved by 1 cm to a new position down the column in a straight line until 19 source positions were measured as shown in figure 1 above.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Nuclear, Particle and Radiation Physics / 78

Isoscalar giant monopole strength in 58Ni, 90Zr, 120Sn and 208Pb

Author: Armand Bahini[1]

Co-authors: Retief Neveling [2]; von Neumann-Cosel Peter [3]; John Carter [4]; Iyabo Usman [5]

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Background: Inelastic α-particle scattering at energies of a few hundred MeV and very-forward scattering angles including 0° has been established as a tool for the study of the isoscalar giant monopole (IS0) strength distributions in nuclei. This compressional mode of nuclear excitation can be used to derive the incompressibility of nuclear matter.

Objective: An independent investigation of the IS0 strength in nuclei across a wide mass range was performed using the 0° facility at iThemba Laboratory for Accelerator Based Sciences (iThemba LABS), South Africa, to understand differences observed between IS0 strength distributions in previous experiments performed at the Texas A&M University (TAMU) Cyclotron Institute, USA and the Research Center for Nuclear Physics (RCNP), Japan.

Methods: The isoscalar giant monopole resonance (ISGMR) was excited in ^{58}Ni, ^{90}Zr, ^{120}Sn and ^{208}Pb using α-particle inelastic scattering with 196 MeV α beam and scattering angles $\theta_{\text{Lab}} = 0^\circ$ and 4°. The K600 magnetic spectrometer at iThemba LABS was used to detect and momentum analyze the inelastically scattered α particles. The IS0 strength distributions in the nuclei studied were deduced with the difference-of-spectra (DoS) technique including a correction factor for the 4° data based on the decomposition of $L > 0$ cross sections in previous experiments.

Results: IS0 strength distributions for ^{58}Ni, ^{90}Zr, ^{120}Sn and ^{208}Pb are extracted in the excitation-energy region $E_{\text{x}} = 9 - 25$ MeV. Using correction factors extracted from the RCNP experiments, there is a fair agreement with their published IS0 results. Good agreement for IS0 strength in ^{58}Ni is also obtained with correction factors deduced from the TAMU results, while marked differences are found for ^{90}Zr and ^{208}Pb.

Conclusions: Previous measurements show significant differences in the IS0 strength distributions of ^{90}Zr and ^{208}Pb. This work demonstrates clear structural differences in the energy region of the main resonance peaks with possible impact on the determination of the nuclear matter incompressibility presently based on the IS0 centroid energies of these two nuclei. The results also suggest that for an improved determination of the incompressibility, theoretical approaches should aim at a description of the full strength distributions rather than the centroid energy only.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Nuclear, Particle and Radiation Physics / 79

Searches for high-mass resonances in the $Z\gamma$ decay mode in Run-2 proton-proton collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector with the integrated luminosity of 139 fb^{-1}

Authors: Phuti Ntsoko Rapheeha[1]; Gaogalalwe Mokgatitswane[2]; Salah-eddine Dahbi[3]; Bruce Mellado[1]

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Corresponding Author: ntsoko.phuti.rapheeha@cern.ch

Searches for new resonances predicted by theories beyond the Standard Model are one of the interesting projects in the physics program of the Large Hadron Collider. This study searches for high-mass spin-0 and spin-2 resonances in the $Z(\ell\ell)\gamma$ final state where the Z boson decays into a pair of oppositely charged muons or electrons. The full Run-2 dataset recorded with the ATLAS detector in the years 2015-2018 with the integrated luminosity of 139 fb^{-1} is used. Upper limits are to be set on the production cross-section times the branching ratio in the mass range of narrow resonances from 200 GeV to 3.5 TeV, assuming spin-0 resonances produced via gluon-gluon fusion mechanism and spin-2 resonances produced via gluon-gluon or quart-antiquark initial states. The expected limits as a function of the resonant mass for the spin-0 and spin-2 resonances are discussed in this study.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Nuclear, Particle and Radiation Physics / **80**

Analysis of Frequentest Study Results in Quantifying Fake Signal Generated in the Training of Semi-Supervised DNN Classifiers

Author: Benjamin Lieberman[1]

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Corresponding Author: benjamin.lieberman@cern.ch

In searches for physics beyond the Standard Model, BSM, machine learning classifiers are used to extract signal from background processes. The use of semi-supervised classifiers allows unlabelled signal events to be classified from labelled background events. This method minimises biases caused by preconceived understanding of the signal. During the training of machine learning classifiers, events can be misclassified. Misclassified events can take the form of fake signals which influence the extent of discovery significance in resonance searches. This study therefore measures the extent of fake signal generated in the training of semi-supervised DNN classifiers using a frequentest methodology. In this study the methodology and results of the experiment are explored using Zɣ final state data, at a fixed centre of mass of 150GeV. The results quantify the extent of fake signal generated as well as account for the probability of observing local excesses, elsewhere within the mass range.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 1 / **81**

Structural Changes of LiXCo2O4 (1 ≤ x ≤ 2) Nanoporous Cathode Materials upon Lithiation

Author: Lisbon Maake[1]

Co-authors: Shibiri Beauty [1]; Phuti Ngoepe [1]; Raesibe Sylvia Ledwaba [1]

[1] *University of Limpopo*

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Spinel cathode material LiCo2O4 exhibit good electrochemical performance when used in energy storage applications. This is attributed to its high surface-to-volume ratios and shortened Li+ diffusion lengths during cycling. However, some possible flaws have constrained the good electrochemical performance. These flaws include structural changes that carry the risk of structural collapse and crack formation during cycling.
Herein, large-scale simulations using molecular dynamics methods were performed to investigate the structural changes of LixCo2O4 (1 ≤ x ≤ 2) nanoporous materials at different lithium concentrations and cell dimensions of 67, 69 and 75 Å. The structures amorphised and recrystallised efficiently under the NST ensemble producing grain boundaries at Li1.75Co2O4 concentration. Furthermore, the increase in lithium concentration in the structures resulted in pore size reduction. Finally, the structures showed great resilience to volume expansion with increasing lithium concentration. This implies that the LixCo2O4 nanoporous materials have the potential to curb the formation of cracks which cause damage to the battery since they are able to expand freely during lithiation.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Astrophysics & Space Science / **82**

On the Perturbations of the Rh=ct Universe

Author: Edmund Kyazze[1]

Co-author: Amare Abebe [1]

[1] *North-West University*

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Decades of astronomical observation have shown that the universe is expanding at an accelerated rate. The standard model of cosmology is the closest we have to a standard theory of gravitation but it fails to adequately describe our universe without the ad hoc introduction of dark energy and dark matter to late-time cosmology and inflation to early-universe cosmology. This has certainly created dilemmas for cosmology and the wider astronomical community, and several alternative cosmological models are being considered at the moment. Current work is limited to the study of background dynamics so a brief overview of the equations that govern the evolution of cosmological perturbations in the $R_h = ct$ model is presented. This model is consistent with observations and has received particular attention in the last few years. Like the ΛCDM model, the $R_h = ct$ model is based on a FLRW cosmology with the cosmic fluid's total energy density ρ and pressure p satisfying the vanishing total gravitational mass condition: $\rho + 3p = 0$. The results derived will be compared to those from the standard model and analysed to see if the model allows for the formation of structure in the universe.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics for Development, Education and Outreach / 83

Surreptitiously feeding education theory to physics students

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Physics is acknowledged to be one of the academic disciplines that students find the hardest, certainly to master but even simply to succeed in. Reasons proposed for this are varied but often incorporate the necessity of working in both the abstract (mathematical) and concrete (physical) realms and the need to transfer knowledge between these realms, while, at the same time, expending great cognitive effort to make sense of the physical world in many, often seemingly different and unrelated, contexts.

I have found the education theory of LCT (Legitimation Code Theory) and its concept of semantic waves to be a powerful explanatory device for this process. I briefly introduce this theory and then give examples of the ways in which I make these processes explicit to physics students during lectures.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics for Development, Education and Outreach / 84

The case for using diagrams to navigate between multiple representations in physics in order to improve conceptual understanding

Authors: Kate Cobbing[1]; Joyce Sewry[1]; Jennifer Williams[1]

[1] *Rhodes University*

Corresponding Author: jennifer.williams@ru.ac.za

Through an interpretation of Greeno's model of the domains of problem-solving and the application of the theory of cognitive load, this paper shows why linking representations through a model aids understanding. The use of a drawing can help physics students to translate more easily between the abstract, concrete and symbolic representations of a physics problem. Physics teachers may find that an awareness of these theoretical underpinnings and their importance in assisting movement between representations informs the way in which they scaffold learning activities.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics for Development, Education and Outreach / **85**

Intentional design of learning material for high school physics teaching based on physics education research

Authors: Kate Cobbing[1]; Joyce Sewry[1]; Jennifer Williams[1]

[1] *Rhodes University*

Corresponding Author: jennifer.williams@ru.ac.za

This paper outlines a structured and intentional approach to the development of learning material for high school physics teaching. This approach is informed by the theory of cognitive apprenticeship and an understanding of cognitive load. The use of worked examples and multiple representations is also promoted. A list of the features that are important in learning material is provided, based on evidence from literature. This may be particularly useful to teachers designing learning material for the first time or for those interested in an approach to material development which is based on Physics Education Research.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 2 / **86**

Probing isothermal and non-isothermal annealing of Sn/Ti bimetallic thin films using Rutherford Backscattering Spectrometry (RBS) as a probing tool.

Author: Keletso Lebesana[None]

Co-authors: Mandla Msimanga [1]; Zakhelumuzi Khumalo [2]; lebogang kotsedi [3]

[1] *Tshwane University of Technology*

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Corresponding Author: keletso77lebesana@gmail.com

Solid phase reaction studies induced by heat treatment processes on Sn-Ti bimetals often lead to changes in microstructural features and enhanced properties and give new insight on the performance of these systems for industry applications. In this study, thin layers of tin and titanium with varying thicknesses of 15 nm and 25 nm were deposited by Molecular Beam Epitaxy (MBE) on a

silicon dioxide substrate. The films were then isothermally annealed at temperatures of 700 oC for 5 hours, 10 hours, and 900 oC for 1 hour in vacuum. Non-isothermal annealing was performed by femtosecond laser irradiation (1030 nm wavelength, 300 fs pulse duration, and 500 kHz repetition rate) at a laser fluence ranging from 76 J/cm2 to 227 J/cm2. The surface morphology and microstructural features of the thin films were investigated by atomic force microscopy (AFM) and scanning electron microscopy (SEM) before and after heat treatment. Rutherford Backscattering Spectrometry (RBS) was used to study the compositional changes of the films. AFM analysis revealed that the surface roughness of the films increased from 5.8 nm to 86.3 nm as the laser fluence increased. RBS also confirmed the increase in surface roughness with laser fluence. However, surface roughness was not observed in the vacuum-annealed samples, which leads to the conclusion that they remained smooth after isothermal annealing under vacuum. Other compositional changes observed were ablation on the laser-scanned samples and the existence of new phases being formed in both vacuum-annealed and femtosecond laser-annealed samples.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Astrophysics & Space Science / 87

NWU Radio Interferometry Commissioning and Verification

Author: Robin Wessels[None]

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The advent of the MeerKAT, a precursor to the Square Kilometre Array (SKA), has driven the need to invest in human capacity development in radio astronomy. The North-West University (NWU) is in the process of commissioning a small four-element radio interferometer. Nooitgedacht Observatory, owned by the NWU, was selected to house the radio telescopes due to the low level of noise present at radio wavelengths in the area. The array consists of four $3.7m$ prime focus parabolic dishes, with a surface accuracy of $0.5mm$, operating at C-band $(6.45 - 6.75GHz)$. The beam size of the individual $3.7m$ telescopes is $43'$, whereas in an interferometer setup, with a fixed maximum baseline length of $180m$, the synthesised beam size is $0.9'$. Each dish has full sky coverage and is mounted with elevation $(0 - 90\ )$ over azimuth $(0 - 360\ )$ motors. The RF front-ends of the telescopes consist of a symmetrical feed horn connected to a C-band LNB $(6.45 - 6.75GHz)$ via coaxial cables. The feed horns have dual polarisation capabilities but are connected for single polarisation observations. The RF back-ends comprise of four receivers that communicate with a pc, wherein each telescope is manually or remotely driven, using proprietary software called RTC. Recently the original receiver back-ends have been replaced by four new wideband receivers that operate in the frequency band $(10MHz - 6GHz)$. This large band of operation will allow for future upgrades with the addition of LNBs that function in different frequency bands. L-band feeds are already in the beginning phase of commissioning, adding to the frequency bands wherein we plan to do observations. Commissioning of the radio telescopes as an interferometer is still an ongoing process. The future aim is to do both single-dish and interferometric observations. In single-dish mode, we will be able to observe very strong MASERs and also perform solar observations. Interferometer mode will enable the study of the morphology of extended objects, such as the Whirlpool galaxy, and radio jet observations.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc.

Nuclear, Particle and Radiation Physics / 88

An alternative explanation of the multi-lepton anomalies at the LHC

Author: Anza-Tshilidzi Mulaudzi[1]

Co-authors: Bruce Mellado [1]; Andreas Crivellin [2]; Guglielmo Coloretti [2]

[1] *University of the Witwatersrand*

[2] *Paul Scherrer Institute, Forschungsstrasse 111, Switzerland*

Corresponding Author: anza-tshilidzi.mulaudzi@cern.ch

In recent years, multi-lepton anomalies have been accumulated by analyzing Large Hadron Collider (LHC) data, pointing towards the existence of beyond the Standard Model (SM) bosons. The data is consistent with a scalar particle S within a mass range between 130 GeV and 160 GeV. A simplified model, the Two-Higgs Doublet plus an additional Scalar (2HDM+S) is used to predict the decay of a singlet scalar $S \to \gamma\gamma$, $Z\gamma$, ZZ and WW and in a recent paper (arxiv:2109.02650), a singlet scalar at 150 GeV was identified, which indicates a scalar resonance S which decays into photons, and, to a lesser extent to $Z\gamma$, in association with missing energy, jets, or lepton. However, we do not see the $S \to ZZ$ signal. Therefore, to allow the scalar to decay into the channel WW and not the ZZ, we look at the Higgs Triplet model where a neutral scalar H^0 can only decay into WW. This study investigates these multi-lepton anomalies by considering the Higgs Triplet Model with a hypercharge of zero (HTM0). It consists of a neutral scalar H^0 that stems from the CP-even component of the Higgs triplet and the two charged scalars $h^{\pm}$ which stem from the charged component of the Higgs triplet. These components come from the mixing between the nonphysical fields of the Higgs doublet and the Higgs triplet.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Theoretical and Computational Physics / 89

Viscous cosmological fluids and large-scale structures

Author: BONANG GEORGE MBEWE[1]

Co-authors: Remudin Reshid Mekuria [2]; Shambel Akalu Sahlu [3]; Amare Abebe Gidelew [4]

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In this work, we present cosmological implications of viscous fluids vis-a-vis background expansion history and large-scale structure formation. The constrained cosmological and fluid parameters which are consistent with available data will first be provided, followed by the study of the growth of matter density fluctuations through the covariant cosmological perturbations formalism. Our preliminary results show the significance of viscosity in the formation of the large-scale structures we observe today.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Astrophysics & Space Science / 90

Analysis of ionospheric storm effects based on GPS and ionosonde data during geomagnetic storms.

Author: Nkosinathi Masango[1]

Co-authors: John Bosco Habarulema [2]; Tshimangadzo Marline Matamba [3]

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Major space weather events may contribute to ionospheric delay where additional noise is introduced into observations of the satellite signal. As a result, the accuracy and reliability of the Global Positioning System (GPS) is compromised. This study aims to conduct an analysis of the ionospheric storm effects using Total Electron Content (TEC) derived from ionosonde and GPS observations during geomagnetically disturbed conditions.

The dataset over a period of 17 years (2005-2022) from co-located ionosonde and GPS receiver over Grahamstown (33° 30'S ,26° 52'E, geographic) will be used. Geomagnetic storm periods selection is based on storm-time criteria of Dst ≤ −30 nT or where Kp > 4. This study will focus on determining the ionospheric storm effects where the ionospheric response are separately studied as established from GPS TEC, bottomside TEC, topside TEC as well as plasmaspheric TEC.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Astrophysics & Space Science / 91

A study of EIA behavior during geomagnetic storms

Author: Avuyile Bulala[1]

Co-authors: John Bosco Habarulema [1]; Tshimangadzo Matamba [1]

[1] *SANSA*

Corresponding Author: bulalaavu@gmail.com

This research study investigates the behavior of equatorial ionization anomaly (EIA) during geomagnetic storms over the African sector (40° S – 50° N and 20° E - 40° E) using a global navigation satellite

systems (GNSS) derived total electron content (TEC) within the period of 2008 to 2013. To identify the geomagnetic storms, the criteria of the disturbance storm time, Dst ≤ -30 nT, and the planetary K Kp ≥ 4 indices are used in the study. To establish the behavior of EIA, the two - dimensional maps of TEC derived from GNSS data are generated during geomagnetic storm periods.
This study also focuses on investigating the role of electrodynamics (vertical E × B drift magnitude) in EIA's variability especially its expansion beyond the crest of about ± 15° towards mid-latitudes during geomagnetic storms. Due to the absence of observed vertical E × B drift data over the longitude sector of interest, we have utilized the equatorial electrojet (EEJ) from ground-based observations based on the well-established differential magnetometer approach. The differential magnetometer approach is used to derive the difference in changes in the horizontal component of the Earth's magnetic field (ΔH) using a magnetometer located at the equator and another one approximately 6° to 9° away from the equator. Specifically for this study, ΔH is derived from a pair of magnetometers at Addis Ababa (0.18°N, 110.47°E, geomagnetic) and Adigrat (6.0°N, 111.06°E, geomagnetic) in Ethiopia.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 1 / **92**

Computational and Experimental Studies on Mn-rich LiMn1.5Ni0.5O2 Cathode Material

Author: Moloko Kgoedi[None]

Co-authors: Tebogo Morukuladi ; Cliffon Masedi ; Noko Ngoepe ; Phuti Ngoepe

Corresponding Author: emmanuel.kgoedi@gmail.com

Abstract
Lithium-ion rechargeable batteries, in particular the cathode materials, are now more essential than ever before as improved, reliable, and effective energy storage systems. Lithium cobalt oxide (LCO), the cathode material now in use, has a reputation for being toxic, expensive, and cobalt-scarce. Due to their accessibility, affordability, and non-toxicity, Nickel Manganese Cobalt (NMC) has been suggested as an alternative cathode material for lithium-ion batteries. In addition, due to their high capacity and improved structural stability, lithium, and manganese-rich composites LiMnNiO2 have gained a lot of interest as potential cathode materials for Li-ion batteries.
In this study, we employed experimental and computational modelling techniques to investigate the stability of manganese nickel oxide LiMn1.5Ni0.5O2 system. The heats of formations indicated that the structure is thermodynamically stable. The results of the lattice parameters, elastic properties and x-ray diffraction agreed with computational and experimental data. A cluster expansion technique generated new thermodynamically stable phases of LiMn1.5Ni0.5O2 system doped with Co and F which could be used for future battery developments.

Keywords: Computational, Doping, Experimental, Structural Properties, Stability.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

Hons

Nuclear, Particle and Radiation Physics / 94

Measurement of the top quark Yukawa coupling from tt kinematic distributions in the dilepton final state

Authors: Cameron Garvey[None]; JAMES KEAVENEY[1]

[1] *University of Cape Town*

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An extraction of the top quark Yukawa coupling (Y_t) from top quark pair production in the dilepton final state using proton-proton collisions recorded by the ATLAS experiment during LHC run 2 & 3 is presented. Corrections from a Higgs boson exchange between the top quark and top anti-quark can produce large modifications to differential distributions near the energy threshold of $t\bar{t}$ production. The kinematic distributions sensitive to these modifications are the invariant mass (m_{tt}) of the $t\bar{t}$ system and the rapidity difference ($\Delta y_{t\bar{t}}$) between the top quarks. This analysis aims to constrain Y_t indirectly using the kinematic distributions of $t\bar{t}$ pair events using the dilepton final states of ee, $\mu\mu$ and eμ channels.

In this talk, the current status of the analysis will be presented, as well as future plans. An event selection scheme has been implemented to optimally select for $t\bar{t}$ events while suppressing background contributions. Although it is possible to reconstruct top quarks, this would introduce large resolution effects and additional systematic uncertainties due to the sensitivity to the reconstruction of the missing transverse momentum. As a result, the kinematic distributions are based on proxy observables that are sensitive to Y_t, namely the m_{tt} and $\Delta y_{t\bar{t}}$. These proxy observables are constructed using the two leptons and the two b-tagged jets. A profile likelihood fit is then implemented to extract a blinded estimation of Y_t using Asimov data including a limited set of systematic uncertainties.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Astrophysics & Space Science / 95

Numerical simulations of the evolution of Astrospheres in the different interstellar conditions

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Astrospheres are bullet-shaped structures formed by the motion of stars through the interstellar medium. This study analyse the impact of the star's outflow parameters, including density, temperature, and magnetic field, on the evolution of the astrosphere using hydrodynamic and magnetohydrodynamical models. The analysis focuses on the compression ratio, velocity and width of the bow shock (outer shell). Hence, the analysis showed that the interstellar medium density affects the astrospheric structure, while the ISM magnetic field can either expand or compress the astrosphere's outer structure. This study also considers various other parameters, such as the time taken to form an astrosphere structure, the effect of the ISM temperature, the mass loss rate, the velocity outflow, and cooling. The results highlight the complex nature of astrospheres and their evolution, and provide a better understanding of these fascinating structures.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Nuclear, Particle and Radiation Physics / **96**

Management of High-Level Radioactive Waste in South Africa

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The National Radioactive Waste Disposal Institute (NRWDI) is mandated by both the NRWDI Act No.53 of 2008 and the South African Radioactive Waste (Radwaste) Management Policy and Strategy (RWMPS) of 2005 to nationally manage the storage and disposal of all classes of radioactive waste. The disposal of Radwaste in stable geological repositories has been recognised as the ultimate world best practice solution and an endpoint for radioactive waste containment and separation from the biosphere. The key issue is that Radwaste is perceived by the public as a danger to society and the environment. The management of High-level Waste (HLW), and particularly Spent Nuclear Fuel (SNF) from Nuclear Reactors still poses a fundamental challenge to the environment mainly due to the presence of long-lived radionuclides like Uranium, Plutonium, and various actinides contained in SNF and associated HLW. We report here on methods and techniques employed to manage HLW and SNF in South Africa as SNF is largely viewed as both a resource and a waste.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 2 / **97**

Resistive Switching property of Cow Milk dispersed with Selenium particles.

Authors: Sonwabile Ntshakaza[1]; Zolile Wiseman Dlamini[None]; Sreedevi Vallabhapurapu[None]; Vijaya Srinivasu Vallabhapurapu[None]

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Scientists are intrigued by the phenomenon of resistive switching in organic materials because of its potential for designing devices with reduced electronic waste footprint. We improved the resistive switching property of organic cow milk films in this study by introducing selenium (Se) particles. We built and tested four devices, each with a different mass per volume % of Se in milk: Ag/milk+Se (0.4)/ITO-PET, Ag/milk+Se (0.8)/ITO-PET, Ag/milk+Se (1.2)/ITO-PET, and Ag/milk+Se

(1.6)/ITO-PET. The resistive switching behaviour of these devices was evaluated. These devices all have distinct current-voltage (I-V) characteristics. The Ag/milk+Se (0.4)/ITO-PET system's I-V hysteresis was found to be weak. Each voltage scan cycle changed the hysteresis properties. The Ag/milk+Se (0.6)/ITO-PET device demonstrated consistent hysteresis, but with substantial signal noise. The Ag/milk+Se (1.2)/ITO-PET device demonstrated consistent hysteresis and decreased noise levels. Before any noise was detected, the hysteresis remained steady for more than 15 cycles. The Ag/milk+Se (1.6)/ITO-PET system had very little hysteresis. This device's behavior was observed to display random variations in current, with no evidence of hysteresis or memory effects. The electron hopping between Se particles is the most likely process, according to the conduction mechanism analysis of Ag/milk+Se(1.2)/ITO-PET.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Applied Physics / 98

ASSESSMENT OF DEMAND CONSUMPTIONS AND POTENTIAL VIABILITY OF INSTALLATION OF BIOGAS DIGESTER IN MELANI VILLAGE EASTERN CAPE, SOUTH AFRICA

Author: Thabiso Mthimunye[1]

Co-authors: Golden Makaka [1]; Patrick Mukumba [2]

[1] *University Of Fort Hare*

[2] *University of Fort hare*

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Abstract: South Africa relies heavily on traditional fossil fuel sources, especially coal. The country initiated the production and distribution of several renewable energy technologies to solve the energy problem in rural areas. Biogas has been proven viable and has begun as a promising technology among several technologies. It has been one of the most successful models for producing clean, environmentally friendly, cost-effective energy sources and has multiple benefits. This paper discusses biogas technology's potential and economic benefits to Melani village households. To measure the demand consumption, onset CTA-A hobo current transducers were installed in three homes to measure the electrical current used in summer and winter. The Data acquisition system has shown that each household consumes an average of 140 kWh of electricity per month. Finally, an analytical life cycle cost analysis of the biogas digester shows that the simple payback period would be approximately 1.1 years.
Keywords: Biogas digester, household, economic, energy, and payback period.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSC

Photonics / 99

Quantum Phase-based Plasmonic Biosensing for Enhanced COVID-19 Detection

Authors: Kelvin Mpofu[1]; Patience Mthunzi-Kufa[1]

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The COVID-19 pandemic has highlighted the urgent need for rapid and sensitive diagnostic tools to enable effective monitoring and control of the disease. In this study, we present an approach to COVID-19 detection by employing quantum phase-based surface plasmon resonance biosensing, which improves the limit of detection (LOD) compared to its classical equivalent. We demonstrate a theoretical framework of a quantum plasmonic biosensor, designed to target the SARS-CoV-2 spike protein with high specificity. In this work we will model and simulate the operation of the biosensor in an ideal noiseless setup as well as in a noisy setup which more realistically resembles the conditions in a lab. Our sensor exploits the advantages of quantum phase sensitivity and surface plasmon resonance to achieve precision level below the shot noise limit. The results show that our quantum plasmonic biosensor outperforms classical counterparts in terms of LOD, offering rapid and precise identification of viral presence at very low concentrations. This work has the potential to lead to more precise optical diagnostic devices and pave the way for more effective public health strategies in combating future pandemics.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / 100

Synthesis and CO gas sensing applications of two-dimensional hexagonal boron nitride nanosheets at different temperatures

Authors: MAGOPA TSHEPHO MCDONALD KEKANA[1]; Thuto Mosuang[2]

Co-authors: Mokete Mahladisa [3]; Lucky Sikhwivhilu [4]

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Abstract

Two-dimensional hexagonal boron nitride nanosheets were synthesised using the wet chemical reaction method. X-Ray Diffraction, Scanning Electron Microscopy, Transmission Electron Microscopy, Fourier Transform Infrared Spectroscopy, Raman Spectroscopy, UV-visible Spectroscopy and Brunauer-Emmett were used to attain the structural properties of the nanomaterials. Each spectroscopic technique affirmed unique features about the surface morphology of the nanosheets. The crystallinity of the nanosheets with the stacking of the B and N honeycomb lattice was validated by the X-ray diffraction. Scanning and transmission electron microscopy disclosed the surface morphology with the number of layers of a planar honeycomb BN sheet. Fourier transform infrared, Raman and UV-vis spectroscopies revealed the formation of the in plane and out of plane h-BN vibrations together with its optical properties. Surface properties were examined with the Brunauer-Emmett approach.

The gas sensing application of the nanosheets was also tested on the carbon monoxide gas. 800℃ fabricated hexagonal boron nitride nanosheets demonstrated good sensitivity towards ppm of CO at 250℃.

Keywords: hexagonal boron nitride, chemical vapor deposition, nanosheets, toxic gases, sensitivity, response.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Consent on use of personal information: Abstract Submission:

Physics of Condensed Matter and Materials Track 1 / 101

Structural and magnetic properties of Mn50Pt50-xNix alloys: A first principles study

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L10 MnPt alloy has attracted much attention recently since it can be easily produced and provides magnetic properties of interest to spintronic applications. According to previous studies, this alloy retains its antiferromagnetism at room temperature. In this study, a first-principles calculations were performed in the framework of density functional theory to identify new spintronic material compositions in Mn-based alloys. By using this method, the structural, electronic structure, thermodynamic, elastic and magnetic properties were determined to track the stability of Mn50Pt50-xNix (x=0, 6.25, 12.5, 18.75, 25) alloys. It was found that the calculated lattice constants of binary systems are in good agreement with available experimental data. According to heats of formation calculations, B2 and L10 Mn50Pt50-xNix alloys are thermodynamically stable when c/a is less than 1.10 suggesting that these alloys can be synthesized experimentally. Furthermore, it was found that the magnetic moments improve with an increase in Ni compositions when the c/a ratio is 1.10 and drops above (c/a>1.10). As a result of these findings, more guided experimental studies can be undertaken on promising Mn50Pt50-xNix alloys for potential use in future spintronic devices.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / 102

Development of TiO_2 nanotube arrays with a modified energy band gap for hydrogen evolution

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Photoelectrochemical water splitting (PECWS) for hydrogen evolution through solar exploitation is a potential alternative way of harnessing energy [1]. TiO_2 is a well-known photocatalyst with exceptionally reliable chemical properties [1]. Highly ordered TiO_2 nanotube arrays prepared by electrochemical anodization have widely been used as photocatalysts due to their unique structure, large specific area, and fast unidirectional charge transfer [1,2]. Pristine TiO_2 has a band gap energy of 3.0 – 3.2 eV, making the material inefficient as a photoelectrode in PECWS, since absorption is limited to the UV region of the electromagnetic spectrum. Narrowing the band gap energy consequently extends its absorption into the visible region, which improves the photocurrent density [2,3].
In this work, the envisaged surface modified TiO_2 photoelectrodes are fabricated through a multi-step electrochemical anodization process. The final anodization step detaches the crystalline TiO_2 nanotube film from the opaque titanium substrate. Thereafter, the film is transferred and pasted onto transparent fluorine-doped tin oxide (FTO) glass. Surface modifications of the nanostructured thin film are achieved through successive ionic layer adsorption reaction (SILAR) to deposit nanostructured metal oxides. The synthesized samples are characterized by X-ray diffraction, SEM, EDS, TEM and UV-Visible spectroscopy.
The results confirm the impregnation of TiO_2 by copper oxide nanoparticles. The optical characterization indicates a red shift in the absorption edge of the CuO/TiO_2 towards the visible light range. The effect of the number of SILAR cycles on the absorption edge has also been investigated in this study. The structural characterization reveals that the loading of CuO on the CuO/TiO_2 nanotubes does not alter the morphology of the nanotubes.
This work demonstrates a facile method to prepare TiO_2 nanostructured heterojunction thin films on a transparent substrate, which could be a promising photoelectrode.
Future work includes optimizing the fabrication process of the photoelectrodes, optical and electrochemical characterization and thereafter, PECWS experiments and hydrogen evolution efficiency measurements.

Key words: TiO_2 nanotube arrays, CuO nanoparticles, SILAR, heterojunction, photoelectrode.

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Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Astrophysics & Space Science / 103

The effects of ion beams on linear and nonlinear ion-acoustic waves in space plasmas

Authors: Mihlali Maxengana[1]; Shimul Maharaj[2]; Ramashwar Bharuthram[3]

[1] *University of the Western Cape and South African National Space Agency (SANSA)*

[2] *South African National Space Agency (SANSA) and University of the Western Cape*

[3] *University of the Western Cape*

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A detailed theoretical investigation is conducted using the Sagdeev pseudopotential formalism to investigate the effects of ion beams on ion-acoustic modes in plasma models with two species of adiabatic ions and one or two (cool and hot) species of electrons which are Boltzmann distributed. One or both ion species are considered to be drifting (beam) components. The linear analysis shows that the slow ion-acoustic modes require a finite value of the beam speed to occur, while the fast ion-acoustic modes are supported in models with or without ion beams. In the one-beam model, the backward propagating slow mode changes direction and couples with the forward propagating slow mode and becomes unstable to the ion beam instability for intermediate beam speeds. "Forward" and "backward" refer to directions which are respectively aligned with or anti-parallel with respect to the beam direction. In the model with counterstreaming beams, the slow modes which propagate in the backward and forward directions which are aligned with the beam directions do not change direction for large values of the speeds of the counterstreaming beams. In the nonlinear regime, the ion-acoustic modes propagate as pulse-like disturbances in potential which are referred to as solitons. Slow solitons with unusual characteristics are found to propagate below the critical speeds corresponding to the phase speeds of the linear waves. On the other hand, negative potential fast solitons coexist with positive potential solitons in the model with two-temperature electrons, in contrast to the model with a single component of Boltzmann electrons for which only positive potential fast solitons are supported.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / 104

Tailoring vanadium pentoxide (V2O5) nanostructure properties to selective detection of nitrogen dioxide (NO2).

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4.University of Sydney, School of Physics, NSW 2006, Sydney, Australia

Abstract

The density functional theory (DFT) method was used to critically investigate the absorption energy of pristine and doped α-V2O5 towards the detection of NO2 gas molecules. The different transition metals, including tungsten (W), copper (Cu), manganese (Mn), tin (Sn), and silver (Ag), were intercalated into α-V2O5 (110) surface using the substitution method to enhance the adsorption energy within the Cambridge Serial Total Energy Package (CASTEP) code. The results show that pristine α-V2O5 lack structural stability and show less negative adsorption energy when the concentration of NO2 molecules increases. α-V2O5 doped with Ag possesses the most negative adsorption energy compared to the pristine and the other dopant. Furthermore, the dopants such as Cu, Ag, and Mn have also enhanced the structural stability of V2O5 at higher concentrations of NO2 molecules. This study paves the way for the experimental fabrication of the most stable and highly selective α-V2O5 doped Ag sensor for selective detection of nitrogen dioxide.

Keywords: V2O5, Adsorption energy, transition metals, gas sensors

Apply to be considered for a student ; award (Yes / No)?:

stu

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Nuclear, Particle and Radiation Physics / 105

Measurements of neutron response functions for a BC-501A liquid organic scintillator between 5 – 66 MeV at the iThemba LABS fast neutron beam facility

Author: Kutullo Maibane[1]

Co-authors: Andy Buffler [1]; Tanya Hutton [1]; Peane Maleka [2]; Zina Ndabeni [1]

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The fast neutron beam facility at iThemba LABS (D-line) offers ns-pulsed neutron fields in the range 5-200 MeV, typically produced via the 7Li(p,xn) or 9Be(p,xn) reactions [1-3], using proton beams from the separated sector cyclotron (SSC). The D-line is currently undergoing a major upgrade and redevelopment towards ISO/IEC 17025 accreditation, including physical modifications of the vault, new instrumentation for neutron metrology and improved beam monitoring and control systems. At present, the standard procedure for characterising the neutron beams and measuring spectral neutron fluence involves a 2" x 4" BC-501A liquid scintillator and a parallel-plate 238U fission chamber (FC) [2,4]. Neutron energy spectra may either be determined directly from time-of-flight measurements using the BC-501A detector, or by unfolding methods if the detector response functions are known sufficiently well over the energy range of interest. The quality of the unfolded neutron energy spectrum is directly related to the knowledge of the detector response to monoenergetic neutrons. For neutron energies below 20 MeV, a detector response matrix can reliably be produced using Monte Carlo radiation transport codes. However, above 20 MeV there are insufficient data regarding the neutron interaction cross sections, and the detector response matrix can only be measured directly.

We report on measurements of response functions in the energy range 5-66 MeV for the BC-501A detector, derived from neutron time-of-flight for the neutron field produced by a 66 MeV proton beam irradiating an 8 mm Li target. Tests of unfolding measured pulse height spectra were undertaken using the unfolding package MAXED [5]. The unfolded neutron energy spectra were experimentally validated by comparing directly with those derived from time-of-flight. The aim is to develop a

portable, scintillator-based neutron detector system for measurements of spectral fluence up to 200 MeV outside of the laboratory environment where time-of-flight is unavailable, whilst maintaining the required standards and traceability.

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Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics of Condensed Matter and Materials Track 1 / **107**

Numerical Simulations Defect-Decorated Carbon Nanotubes under Pressure

Authors: Robert Warmbier[1]; Xolani Maphisa[2]

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Carbon nanotubes (CNTs) are amongst the strongest materials known with very high tensile strength and Young's modulus. Unfortunately the ideal parameters primarily refer to single nanotubes. In amorphous materials and non-twisted bundles the macroscopic strength is limited by the relatively weak van der Waals interaction between the tubes.
In recent years researchers have tried to modify CNT-based materials in various ways, including irradiation to create defect-decorated CNTs. In this paper we present Density Functional Theory and Molecular Dynamics simulations of defect-decorated CNTs. We show that even small fractions of extra defects in the material can lower the collapse pressures significantly. The extra defects also facilitate deformations into oval and race-track shapes at lower pressures. The interplay between defect-decorations and pressures further allows for local morphological changes, including CNT-interlinking, which do not lessen the strength of CNTs further, but might improve other material properties.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / **110**

Optimization of multi-walled carbon nanotubes for improved heat transfer

Author: hlabane Beauty Masolo[None]

Co-authors: David Motaung ; Solethu Nkosi ; Mmantsae Diale [1]

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Abstract

Carbon nanotubes (CNTs) are excellent for heat transfer in fluids due to their high thermal conductivity of (>3000 W/mK) and specific heat capacity of (49.11 W/m2 K). They are preferred in industry due to their high thermophysical properties. In this study, CNTs were synthesized using chemical vapour decomposition (CVD). Morphology and structure of the CNTs were revealed using scanning electron microscopy (SEM) and transmission electron microscopy (TEM), allowing for the measurements of individual CNTs inside and on the surface of composite materials. Dynamic light scattering (DLS) measured the Brownian motion of the macromolecules in the carbon nanotubes fluid which have been found to be 2-10 nm long. Nanofluids stability has been analysed using zeta potential, UV–vis spectroscopy characterize the dispersion effect of carbon nanotube suspensions. For more stability of multi-walled carbon nanotubes (MWCNTs)/water nanofluids, surface active reagent such as polyvinylpyrrolidone (PVP) was utilized. The results shows that heat transfer efficiency in fluids is improved by MWCNTs, and confirms that MWCNTs are promising nanoparticle material in nanofluids and hence predict their wide application in heat transfer industry.

Keywords: Carbon nanotubes, Heat transfer, Brownian motion, Nanofluids.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

Msc

Nuclear, Particle and Radiation Physics / 111

Feasibility Study to Search for Additional Scalars at Future e^+e^- Colliders

Authors: Karabo Mosala[1]; Pramod Sharma[2]; Mukesh Kumar[3]; Bruce Mellado[4]; Salah-Eddine Dahbi[3]; Prince Siboniso Ntimeni[1]; John Michael Statheros[1]

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We presents a full simulation study of the production of a scalar (M_S) using $e^+e^- \rightarrow ZS$ at the future e^+e^- colliders. We consider the events in which a Scalar recoils against a Z boson decaying into a pair of muons or electrons at $\sqrt{s} = 250$˜GeV. We evaluate the statistical precisions of the Scalar mass m_S measurement at the future e^+e^- colliders in the $Z \rightarrow \mu^+ \mu^-$ channel and provide the extension to additional $Z \rightarrow e^+ e^-$ channel. For the whole mass range, $M_S = 90 - 200$˜GeV, the observed limit on the cross section is weaker than expected. Furthermore, at ≈ 95˜GeV the limit is weakest and a new scalar subsequently decays leptonically with a cross section ≈ 0.5 pb indistinguishable over the Standard Model hypothesis. We use Deep Neural Network (DNN) as a machine learning technique to provide discrimination at ≈ 95˜GeV.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Nuclear, Particle and Radiation Physics / **112**

Searching for Low-Mass Resonances Decaying into W Bosons

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The Brout Englert-Higgs boson, discovered at the LHC, provided the final piece of the puzzle for the Standard Model (SM) of particle physics, which has undergone extensive testing and verification both at the precision and at the high energy frontier. However, this does not exclude the existence of additional scalar bosons as long as their role in the breaking of the SM electroweak gauge symmetry is sufficiently small. In fact, searches for new resonances at the LHC, including additional scalar bosons, have been intensified since the Higgs boson discovery. While the LHC experiments ATLAS and CMS did not observe unequivocally the production of such a new particle, interesting hints for a new scalar with a mass around 95 GeV and 151 GeV arose, as well as anomalies in multilepton final states. The latter include hints for the enhanced nonresonant production of different-flavour opposite-sign di-leptons which can be explained by the decay of a neutral scalar with a mass between 130 GeV and 170 GeV decaying into pairs of W bosons. In this study, we recast and combine the CMS and ATLAS analyses of the Standard Model Higgs boson decaying to a pair of W bosons in order to search for low-mass resonances in this channel. In the first part of the analysis, we consider a new neutral scalar S with mass m_S at the LHC, that is produced directly via gluon fusion and decays dominantly into a pair of W bosons (one of which can be off-shell) which subsequently decay leptonically. Next, we use a simplified model to advocate this low mass resonances search as well as the multilepton anomalis by the decay of a neutral scalar H (270 GeV) into a pair of lighter one S (150 GeV) and i.e. $H \to SS$, as realized within the 2HDM+S model.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / **113**

Confocal Raman and AFM Characterization of Mesoporous Titania Electrode Substrates for Perovskite Solar Cell Applications

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Confocal microscopy is a technique of choice for high resolution imaging of a wide range of sample surfaces. It also plays a vital role in the optical sectioning of imaged materials for 3D reconstruction. Similarly, atomic force microscope (AFM) is renowned for its capability in evaluating the local properties of different samples precisely down to atomic scale. The amalgamation of AFM with Raman spectroscopy is beneficial in supplying a more comprehensive information on the material properties, in addition to providing ultra-high resolution micrographs of various samples ranging from silicon, fullerenes, polymers, composites, perovskites and many others. Perovskite materials exhibit specific characteristics that distinguish them from other solar cell materials such as low excitonic binding energy, ferroelectric properties, high dielectric constant and absorption coefficient etc. These properties have enabled perovskite solar cells (PSCs) to be renowned as promising alternative technology for silicon-based photovoltaic technology. Intensified efforts are made to improve the stability and commercialization of PSCs through the integration of optimizing additives, effective electron transporting material (ETL) and hole transporting material (HTL) in the perovskite material. In the present work, the interfacial physical properties of mesoporous titania electrode substrates and information on the depth profiles of embedded structures were investigated for prospective applications in perovskite solar cells. This was achieved by obtaining mapped 2D Raman images of specific surfaces on the mesoporous titania electrode and comparing them with their respective morphological information which was extracted through tapping mode AFM technique. Results contained in this work are aimed at improving understanding of the material properties through visualization of both chemical and structural information over a defined area of interest on the sample. The relationship between phase transitions as derived from the micrographs is expected to provide vital interpretation on chemical activities in the mesoporous substrates.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / 114

Intrinsic defect interactions in a monolayer silicene: An ab-initio DFT study

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Silicene is a two-dimensional structure of silicon which has been synthesized experimentally. It is mechanically and thermally stable and possess the possibility of being easily integrated into the existing silicon technology, hence its importance in semiconductor device technology. However, the performance of any semiconductor material is dependent on the type, stability, and interactions

between the defects as well as the mobility of defects that are intrinsic to it. Using the density-functional theory (DFT) approach, we study the stability, electronic and magnetic interactions between various vacancy defect configurations in silicene. We provide a deeper understanding of fundamental properties of defective silicene containing vacancies and also demonstrate how the presence of vacancy-like defects may impact on the potential applications of silicene in such fields as spintronics and valleytronics.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics of Condensed Matter and Materials Track 2 / **115**

Interaction of methanoic acid with arsenopyrite (001) and sperrylite (100) surfaces: A DFT-D and atomistic simulations studies

Author: Thapelo Ntobeng[None]

Co-authors: Mofuti Mehlape [1]; peace prince mkhonto [2]; Phuti Ngoepe [2]

[1] *University Of Limpopo*

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Corresponding Author: thapelosegoarihle@gmail.com

The study of the surface chemical behaviour of sulphides and arsenides is very crucial in the field of mineral processing and ore beneficiation. The dispersion-corrected density functional theory (DFT-D) and atomistic simulations were employed to investigate the adsorption behaviour and mechanism of methanoic acid on arsenopyrite (001) and sperrylite (100) surfaces. It was found that methanoic acid preferred to adsorb on the Fe and Pt sites than As and/or S atoms on arsenopyrite and sperrylite, respectively. The adsorption energy of methanoic acid on arsenopyrite was −62.52 kJ/mol, while the adsorption on sperrylite gave −20.40 kJ/mol from DFT-D simulations. It was clear that methanoic acid preferred the arsenopyrite than sperrylite mineral. This study predicted that it is easy to remove limescale such as calcium carbonate (CaCO3) on sperrylite without methanoic acid adsorbing to some extent on the surface, while on arsenopyrite the methanoic acid may be adsorbed. Similar findings were obtained from atomistic simulations and therefore these methods can be used concurrently to understand surface reactivity of these minerals.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / **116**

Combining large radio and optical astronomical surveys: exploring the MeerKAT Galaxy Cluster Legacy Survey

Authors: S.J.J. Nel[None]; SI Loubser[None]

We are entering an era of large radio and optical astronomical surveys, particularly for the Southern Hemisphere. One challenge is to effectively combine and cross-match source catalogues from surveys in different wavelengths, thereby maximising the science impact of surveys. We use the Likelihood Ratio method to cross-match compact source catalogues extracted from the MeerKAT Galaxy Cluster Legacy Survey (MGCLS) with optical sources detected in the Dark Energy Camera Legacy Survey (DECaLS). These matched catalogues can now be further explored for various science applications, and to possibly improve the cross-matching method for future surveys. For this presentation, we contrast and test two different methods to evaluate the "Reliability" and "Completeness" of the cross-matching method and the resulting catalogues to determine which method is better suited for optimally combining large radio and optical surveys.

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Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

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Nuclear, Particle and Radiation Physics / 117

Probing the parameter space of Scale Invariant Scotogenic Model at the LHC

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In this talk we explore the scale invariant (SI) scotogenic model in the context of anomalies observed in various multi-leptonic final states at the Large Hadron Collider (LHC). This model is vary well known to accommodate dark matter (DM) requirements in association with scalar sector. In a classically SI framework this model is also motivated by neutrino mass and DM. This model is an extension of the standard model (SM) by a real singlet, an inert scalar doublet and three Majorana singlet fermions. And hence a large parameter space with neutral and charged scalars in association with heavy neutrinos allows various production and decay modes in leptonic final states with missing energy. We use this model to search beyond the SM resonance(s) compatible with observed signal(s) in the scalar sector at the LHC.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Nuclear, Particle and Radiation Physics / 118

W-boson mass in beyond the standard model

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Following a discussion on W-boson mass observed at the CDF and ATLAS, we explore the parameter space allowed in 2HDM+S model. Further the model parameter space are constrained through vector-like leptons via muon g-2 dataset. We show our results for additional scalar mass fixed to $m_S \approx 96$ and 150 GeV keeping the standard Higgs-boson mass at 125 GeV in all four types of 2HDM+S model. The chosen mass of the singlet scalar is motivated by the excesses seen at the CMS and ATLAS data in proton-proton collisions at the Large Hadron Collider.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Astrophysics & Space Science / **119**

Sunspot Number, Solar Flares and Atmospheric Gravity Waves

Author: Matsobane Alex Mothibi[1]

Co-author: John Bosco Habarulema [2]

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[2] *South African National Space Agency*

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The purpose of the experiment was to determine the effect the sunspot number would have on the number of solar flares. The hypothesis stated that as the sunspot number increased, the number of solar flares would also increase during the same time period. With the ability to predict the occurrence of solar flares from sunspot activity, it may be possible to prevent the damage to power grids and satellites caused by solar flares. A catalogues solar flares, geomagnetic activities and It's driver have been created to assist this project. The catalogue starts from 2000 January to 2022 December. From the study reveal that there are remarkable differences on the relationship between sunspot number (SSN) and M- and X- solar flares during the solar cycle phases of low (-activity), high (-activity), ascending, and descending. For future studies the catalogue will be used to assess the atmospheric gravity waves at low latitude during disturbed times (during geomagnetic storms only, solar flares only and geomagnetic storms + solar flares)

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / **120**

The Shape of 36Ar in its first 2 plus state

Author: Ntokozo Radebe[None]

Co-authors: Nico Orce [1]; Sifiso Senzo Ntshangase [2]

[1] *University of the Western Cape*

[2] *University of Zululand*

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In 1970, a Coulomb excitation experiment was done in order to determine Spectroscopic Quadrupole moment of Argon-36 (36Ar) in its first excited state which has the total angular momentum of 2 and a positive parity. The 36Ar ion beam was bombarded towards a stationary Lead-206 (206Pb) target The Spectroscopic quadrupole moment was determined to be 0.11 ±0.06 e.b. At the time of the experiment, the distance of closest approach between the nuclei surfaces was 4.3 fm (fentometer) which is less than minimum distance of 6.5 fm for the experiment to be from nuclear force interference. The Coulomb excitation experiment of 36Ar was conducted for a month at the ithemba LABS facility located at the Western Cape. The objective was to determine the Spectroscopic Quadrupole moment of 36Ar in its first excited state. The 36Ar ion beam was accelerated towards a 1 mg/□cm□ˆ2 thick 194Pt (Platinum-194) stationary target. The gamma rays emitted by the de-excited nuclei were detected using the AFRODITE, which consist of eight clovers and each clover has four 50×70 □mm□ˆ2 high purity Germanium crystal. The backwards scattered ion beam was detected by the double-sided CD-shaped silicon particle detector. The information about the gamma rays that were in coincidence with the scattered particles will be analysed using MIDAS MTsort offline. The doppler-corrected 36Ar and non-doppler corrected 194Pt spectra peaks acquired from MIDAS MTsort along with other spectroscopic information was analysed by the GOSIA program and from it, the Spectroscopic Quadrupole moment will be determined.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Astrophysics & Space Science / 121

Investigating the solar differential rotation rate by sunspot tracking using terrestrial solar observations.

Author: Calmay Lee[1]

Co-authors: Petrus Johannes Steyn [2]; Martin Snow [3]

[1] *North-West University*

[2] *NWU Centre for Space Research*

[3] *South African National Space Agency*

Corresponding Author: calmay.lee9@gmail.com

The Centre for Space Research (CSR) at the North-West University (NWU), South Africa, commissioned a solar telescope in 2021. The weather in Potchefstroom, South Africa, is ideal for solar observations for the biggest part of the year, especially during the dry winter months. The first science application of the solar telescope was investigating the differential rotation rate of the Sun. The solar differential rotation rate is known to be latitudinally dependent. In this study, the photospheric rotation rate is experimentally determined by tracking multiple active regions over successive days using a dedicated hydrogen-alpha solar telescope. The observational campaign runs over a period of 46 days between 15 August and 14 October 2022. A total of 29 active regions are studied. The results of this study are compared to three published models. On average, a faster rotation rate is observed

when compared to accepted model predictions. Factors influencing the observational data are investigated, such as the number of observations, the area of a single active region (containing multiple sunspots), as well as the location of each active region with respect to the solar limb.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

Hons

Poster Session 1 / **122**

Investigation of the fundamental interactions of the PtSb2 Surface with the MBTK molecule

Author: ivyn ndhlovu[1]

Co-authors: Phuti Ngoepe [2]; Seshupo Mangwejane [2]; Peace Mkhonto [2]

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[2] *University of Limpopo*

Corresponding Author: ivyn8012@gmail.com

Collectors play a key role in determining a minerals floatability behaviour. Variations in chain length have a specific effect on xanthate collectors, which continue to be the most versatile collector for the bulk of minerals, this leads to better recovery rates. This study investigates adsorption energies, bonding behaviour and the interaction of the mercaptobenzothiazole (MBTK) with the platinum antimony mineral surfaces: (100), (110) and (111) surfaces. Following the three surfaces optimization, we identified the most stable surface and calculated the adsorption energy. We found that the most exothermic was the (110) surface with a greater adsorption energy of -6.932 kJ/mol, the (100) surfaces produced an adsorption energy of -6.838 kJ/mol and the (111) surface produced an adsorption energy of -0.365 kJ/mol thus shows that the (MBTK) molecule was mostly preferred on the (110) surface.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

Hons

Poster Session 1 / **123**

Thermal conductivity enhancement in gold decorated graphene nanosheets in ethylene glycol based nanofluid

Authors: Makhangele Mbambo[1]; Thembinkosi Nyawo[1]

Co-authors: Bongani Mtshali [2]; Zakhele Khumalo [3]

[1] *Cape Peninsula University of Technology*

[2] *iThemba LABS*

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ABSTRACT

We report on the synthesis and thermal conductivity of gold nanoparticles (AuNPs) decorated graphene nanosheets (GNs) based nanofluids. The GNs-AuNPs nanocomposites were synthesised using a nanosecond pulsed Nd:YAG laser (wavelength = 1064 nm) to ablate graphite target followed by Au in ethylene glycol (EG) base fluid to obtain GNs-AuNPs/EG hybrid nanofluid. The characterization of the as-synthesised hybrid nanofluid was carried out using high-resolution transmission electron microscopy (HR-TEM), scanning electron microscopy (SEM), energy dispersive X-ray (EDX), X-ray diffraction (XRD), Raman spectroscopy, Fourier transform infrared (FT-IR) spectroscopy and ultraviolet-visible spectroscopy (UV-Vis). The thermal conductivity of the as-synthesised hybrid nanofluid was measured by a guarded hot plate (GHP) apparatus at different temperatures in the range 25 – 45 ℃. The characterization of the as-synthesised GNs-AuNPs/EG hybrid nanofluid confirmed a sheet-like structure of GNs decorated with crystalline AuNPs with an average particle diameter of 6.3 nm. The thermal conductivity analysis showed that GNs-AuNPs/EG hybrid nanofluid exhibits enhanced thermal conductivity of 0.41 W/mK compared to GNs/EG (0.35 W/mK) and AuNPs/EG (0.39 W/mK) nanofluids, and EG base fluid (0.33 W/mK). The enhanced thermal conductivity of the hybrid nanofluid is due to the synergistic effect between AuNPs and graphene sheets which have inherent high thermal conductivities. GNs-AgNPs/EG hybrid nanofluid has the potential to impact on enhanced heat transfer technological applications.

KEYWORDS: Laser ablation; graphene nanosheets; Au nanoparticles; Ethylene glycol; Thermal conductivity; Nanofluid

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Theoretical and Computational Physics / 124

First-principles study on the effect of Pt addition on the stability of B2 Ti50Ru50 – a supercell approach

Authors: Bongani Ngobe[1]; Maje Phasha[2]; Mahlaga Molepo[3]

[1] *WITS and MINTEK*

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[3] *University of the Witwatersrand*

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Keywords: Advanced structural materials, First-principles calculations, Density functional theory (DFT), Phase stability and Phase transition

Abstract: The discovery of new advanced structural materials to meet the aggressive evolving engineering structural demands can be achieved through the integration of computational thermodynamics and validated experimental activities to optimize the existing materials. Nitinol, Ti50Ni50, is a commercial shape memory alloy (SMA) widely used in structural applications is known to possess shape memory effect and excellent super-plasticity. Materials that display such unique structural properties are usually referred to as SMAs, with a tendency of recalling their prior crystal structure and properties if subjected to a conducive environment such as temperature. Though Nitinol

is widely known as an alloy with shape memory effect (SME), it has drawn back such as being limited to low-temperature structural applications. So any advanced structural materials that could overcome Nitinol's structural application's limitation stand a good chance to be considered as high-temperature shape memory alloys (HTSMAs). This SME is driven by a diffusionless phase transition, from an ordered high-temperature B2 phase to disordered low-temperature martensite phases (L10/B19/B19'), present in CsCl compounds. Whilst Ti50Ru50 also consist of B2 at high-temperature, it remains ordered with no phase transition to 0 K. Owing to platinum's nobility and excellent malleability, this work employed a supercell (SC) approach to pin-track B2-Ti50Ru50-xPtx ternary compositions with the prospect to stimulate SME on stable B2-Ti50Ru50 by substituting some of Ru atoms with Pt atoms. In pursuit of such advanced structural materials with SME, we evaluated the thermodynamic, mechanical, electronic and lattice dynamic stability using first-principles calculations.

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YES

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / **126**

V2O5 nanostructures for gas sensing: doping, and low temperature detection of Methanol, Ethanol and NO2 with superior response of H2S

Author: Mick Molukie Mokwena[1]

Co-authors: Olatunbosun Nubi [2]; Amos Akande [3]

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[2] *University of Limpopo*

[3] *University of Sydney*

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A facile reflux method was used to synthesize the undoped and Au-doped V2O5 nanoparticle powder samples at concentrations ranging from 1 wt% to 5 wt%. XRD, SEM, BET, FTIR and UV-Vis analysis revealed a change in morphology from spherical to nanorod-like nanostructures upon doping with the gold. The Au-doped V2O5 nanostructures tend to increase in surface area, and also become more crystalline with increase in Au concentration. The V2O5 nanostructures were found to have a larger optical band gap when compared with bulk V2O5. The undoped V2O5 sample was tested against ethanol (C2H5OH), hydrogen sulphide (H2S), methanol (CH3OH) and nitrogen dioxide (NO2), at low temperatures ranging from 25oC to 150oC and concentrations from 5 ppm to 100 ppm. A high response of 130 towards 100 ppm H2S at 75oC, was exhibited by the undoped sensor. The sensitivity of the V2O5 sensor in the low temperature range of 25oC to 150oC was found to follow the sequence of H2S > C2H5OH > CH3OH > NO2.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / 127

Cluster expansion calculations on the discharge product of magnesium-ion batteries

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Co-authors: Phuti Ngoepe [2]; Cliffton Masedi [2]

[1] *UL*

[2] *University of Limpopo*

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Magnesium batteries have poor cycle performance, which limits their commercial use. In magnesium batteries, sulphur (S) performs poorly and reduces the battery's performance; however, when selenium (Se) is added, the issue is improved and the material's energy density is enhanced. Therefore, in this study, cluster expansion technique was employed to determine phase changes of mixed MgSc2S1-xSex, MgY2S1-xSex, and MgIn2S1-xSe systems, which then generated 97, 61, and 12 new mixed phases, respectively. Furthermore, the potential of Se, a d-electron possessing periodic table element with excellent electrical conductivity, as an electrode material for rechargeable magnesium batteries is explored. The systems created a miscibility gap, leading to the introduction of Monte Carlo simulations. Monte Carlo simulations produced thermodynamic properties for Se concentrations obtained from cluster expansion, and it demonstrated that all the systems are phase separating at 0K. Temperature was varied and the systems changed to mixed systems at an approximately 250K-400K range. Finally, Monte Carlo simulations yielded consistent results on phase separation and high-temperature behaviour for all the systems at 50% sulphur and selenium.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics of Condensed Matter and Materials Track 1 / 128

Dual-Site Loading and Characterization of Cobalt Ferrite Nanostructures

Author: Sunday Ogundipe [1]

Co-authors: Ntokozo Cebekhulu [1]; Solethu Nkosi [2]; Neerish Revaprasadu [1]; Ceboliyazakha Ndlangamandla [3]

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[2] *University of Limpopo*

[3] *University of zululand*

Corresponding Author: ogundipesunday6@gmail.com

Dual-site loaded cobalt-ferrite spinel nanostructures with chemical formula Co1-2xNixMnxFe2-yCeyO4, where $0 \leq x = y \leq 0.3$, were successfully prepared via glycolthermal route. The final products of the appropriate sites loading are CoFe2O4 (dried naturally), CoFe2O4 (dried with Infrared lamp), Co0.8Ni0.1Mn0.1Fe1.9Ce0.1O4, Co0.6Ni0.2Mn0.2Fe1.8Ce0.2O4, and Co0.4Ni0.3Mn0.3Fe1.9Ce0.3O4. The structure, surface morphology, surface area, elemental composition and optical analysis were carried out by X-ray diffraction (XRD) and high resolution transmission electron microscopy (HRTEM), scanning electron microscopy (SEM), Brunauer-Emmett-Teller (BET), X-ray photoelectron spectroscopy

(XPS), and UV–vis spectroscopy (UV). XRD results showed the cubic crystal structure and spinel formation of the samples; HRTEM confirms the crystallinity of the samples. SEM revealed the nano-spherical nature of the samples. BET results showed that the samples are mesoporous. The presence of the constituent elements of the Co1-2xNixMnxFe2-yCeyO4 spinel was verified by XPS. The band gaps of the samples estimated from the Tauc plot were found to be between 1.88 and 2.55 eV.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Photonics / 129

Majority Voting Algorithm for TB Detection: Machine Learning Approach

Authors: Nkgaphe Tsebesebe[1]; Kelvin Mpofu[2]; Sphumelele Ndlovu[2]; Patience Mthunzi-Kufa[2]

[1] *University of Cape Town*

[2] *CSIR*

Corresponding Author: ntsebesebe@csir.co.za

Mycobacterium tuberculosis (Mtb) is an intracellular pathogen that has evolved defense mechanisms to evade the human immune response, allowing it to persist indefinitely in the host. The bacterium primarily targets the human lungs and produces the contagious disease tuberculosis (TB). Although the bacteria attack the lungs, TB can spread to other parts of the body such as the kidneys, bones, and brain. Tuberculosis can be fatal if not properly treated and it has already claimed the lives of many people throughout the world. Hence, early detection and treatment of the diseases are essential to improving the likelihood of a full recovery. Machine learning algorithms (ML) have shown great potential to provide more accurate diagnostic results while saving money and human lives. However, the technique can be accurate to a certain degree and improvements are required. In this work, a combination of machine learning algorithms (i.e., a convolutional neural network, a support vector machine and decision tree algorithms) use majority voting to classify chest X-ray images into infected and noninfected. The performance of the individual algorithms is optimized by hyperparameter techniques such as grid search; therefore, the voting system made of the three algorithms achieves an accuracy of 99% in classifying 800 (200 healthy and 600 TB-infected) chest X-ray images. The system classifies the TB-infected images by 98% and non-infected images by 100% providing high precision and recall. As such, the voting algorithm in this study can be applicable to point-of-care settings and has the potential to serve as a supplement to conventional illness detection techniques used in the medical industry.

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Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Nuclear, Particle and Radiation Physics / 130

Analysis of Trace Elements in Some Traditional Medicinal Plants and Developing Nuclear Forensic Signature

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[1] *North West University (Mafikeng), postdoctoral research fellow at CARST*

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Medicinal plants are the most sensitive factors that show the interaction between human activities and the ecological environment.The aim of this study is developing the therapeutic trace elements and nuclear forensic signature in medicinal plants of East Gojjam using nuclear techniques as tools. The samples from medicinal plants were accurately weighed and transfered into the irradiation as well as digestion vessel, and introduced into a nuclear reactor and inductively coupled plasma mass spectrometry.Then the induced activities of the radionuclides were counted by calibrated detector. The results were discussed with careful references (NIST 81 materials) to establish role of essential elements in the physiology and patholgy of human life. The data obtained on the elemental concentration of the medicinal plants will be useful in deciding the dosage of the traditional drugs prepared from these medicinal plants. Nuclear forensics involves the interpretation of elemental contents (Na, K, Mn, Fe, Co, Zn, Se, Br, La, Sm,As and Eu) of medicinal plants and will accquire understanding of production of radioactive isotopes by irradiation, detection and identification methods. Lead isotope ratios (204Pb/206Pb, 208Pb/206Pb and 207Pb/206Pb) and Rare Earth Elements (REE) also show significant spatio-temporal variability along the study areas.The traditional knowledge of plants for medicinal purpose has been passed from generation to generation orally.The present research work will be helpful to traditional doctors, scholars, budding students and scientists to share their research findings with the global experts in the areas of traditional medicines.
Keywords: inter-elemental correlations, traditional doctors, indigenous use, rural areas

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / 131

Investigation of the structural, elastic and vibrational stability of PtTe, PtTe2, Pt2Te3 and Pt3Te4 tellurides structures

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Co-authors: PEACE MKHONTO ; BRADLEY NEMUTUDI ; PHUTI NGOEPE

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Platinum tellurides are platinum group minerals (PGMs) predominantly found in the Platreef Bushveld Complex of South Africa, which is one of the leading countries with highest percentages of PGMs. Besides being the important carriers of precious metals, telluride minerals are minor constituents in an ore deposits from a wide diversity of geological environments and they are of significant economic importance. In this study Vienna Ab-initio Simulation Package (VASP) code was employed to investigate the structural, thermodynamic, elastic and vibrational properties of PtTe, PtTe2, Pt2Te3 and Pt3Te4.The calculated lattice parameters agreed well with the available experimental data. In addition, the calculated heats of formation predicted that PtTe2 was more stable than the PtTe, Pt2Te3 and Pt3Te4. The elastic constants indicated that PtTe, PtTe2, Pt2Te3 and Pt3Te4 were mechanically stable. It was observed that the PtTe was ductile, while PtTe2, Pt2Te3 and Pt3Te4 were brittle. The phonon dispersion curves showed no soft modes for PtTe, PtTe2 and Pt3Te4 suggesting stability, while Pt2Te3 was unstable due to the presence of vibrations in the negative frequency. The total density of states (TDOS) for all the structures showed a metallic behaviour due to absence of a band

gap. These findings gave more insights on the stability of these minerals for future studies that will include surfaces in particular for PtTe2 which is dominates in the Platreef Bushveld Complex.

Apply to be considered for a student ; award (Yes / No)?:

YES

Level for award;(Hons, MSc, PhD, N/A)?:

HONS

Nuclear, Particle and Radiation Physics / **132**

Application of IAEA Radio-Photoluminescence Glass Dosimeter for Radiation dose monitoring

Authors: Manny Mathuthu[1]; Seepamore Dithole[2]; Vincent Maselesele[3]

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[2] *National Metrology Institute of South Africa*

[3] *Steve Biko Academic Hospital, Dr Savage Road, Pretoria, 0001, South Africa*

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Radio-Photoluminescence Glass Dosimeters are solid-state detectors, which use the accumulation of radiation counts technique to measure the amount of radiation dose acquired. In this study, they were applied to measure the personal dose equivalent from two gamma radiation sources, i.e Co-60 teletherapy source, and Cs-137 low-level radiation source. Two reference detectors (0.6 cc farmer chamber and 1000 spherical ionization chamber) were used to determine the reference dose measurements, and the RPLGD was introduced as the Device under test using the substitution method. The reference measurements of absorbed dose to water and air kerma were made. Calibration coefficients for both sources were used to convert the measurements from air kerma (Grey) to a personal dose equivalent (Sievert). The RPLGD measurements comprised determining the following quantities; sensitivity, accuracy, reproducibility, fading effect, energy dependence, dose range, and the uncertainty budget. It was noted that RPLGDs are user friendly and reliable for personal radiation dose monitoring. They can be read multiple times without losing radiation signal and can reproduce the same signal up to an accuracy of 3 %. Correction factors were used to adjust for any anomalies in the measurements of all quantities. The uncertainty budget of the RPLGDs in both radiation sources did not exceed 5 % and it included all the significant contributors that affected the measurements and maximum expanded uncertainty. This was at a confidence level of 95 %.

Apply to be considered for a student ; award (Yes / No)?:

NO

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Astrophysics & Space Science / **133**

Dark Matter annihilation and the termination of the Martian geodynamo

Authors: Javeria Makda[1]; Geoffrey Beck[2]

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In this work we derive limits on the WIMP-nucleon scattering cross-section by comparing the potential heat flow within the Earth from Dark Matter capture and subsequent annihilation to the observational value. This effect has been argued previously in the literature to provide a potential link to mass extinction phenomena on Earth. However, we focus on whether additional heat-flux from dark matter annihilations within the Martian core could have affected the decay of its geodynamo, and thus precipitated its magnetic field loss. We determine that Xenon1T limits on the WIMP nucleon cross-sections do not allow sufficient heating to significantly affect either Earth or Mars. We then use this to determine the local dark matter density that would support a significant effect given these limits. In addition, we have extended previous work on this topic by including resonant collisional effects, considering the impact of Xenon1T limits, and by considering possible effects on the evolution of the Martian geodynamo.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / **134**

Phase stability of calcium manganese oxide (CaMn2O4) polymorphs cathode materials in calcium ion batteries.

Authors: OSWALD ROBERTS[None]; NDANDULENI LETHOLE[None]

Corresponding Author: 201716358@ufh.ac.za

The demand for energy storage devices with high energy density has increased with the development of renewables occurring. Calcium ion batteries (CIBs) have gained attraction due to their abundance, high energy density, low cost, and low risk. Supercapacitors and Batteries are the currently used energy storage devices with Batteries being the dominant/most used. This study presents computational calculations that were carried out on the structural, thermodynamics, electronic and mechanical properties for CaMn2O4 polymorphs. The computational method used the density functional theory (DFT) that is imbedded in the CASTEP code in Material Studio. Since we were dealing with transition metal oxides, we had to employ the Hubbard U-correction to take care of the highly-correlated electrons in the d-orbital of the Mn atoms. The lattice parameters found were in good agreement with available experimental results validating the approach taken. The heats of formation are both negative which suggest that the structures can be synthesized experimentally. During the analysis of the DOS the considered CaMn2O4 polymorphs showed a relatively poor conductivity and can be classified as semi-conductors. Furthermore, Pbca-CaMn2O4 has lower states around the Fermi level as compared to Pbcm-CaMn2O4, suggesting that the Pbca-CaMn2O4 polymorph is more stable. This is consistent with the calculated heats of formation.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics of Condensed Matter and Materials Track 1 / 135

Gas sensing performance of pristine and modified Ga2O3 nanostructures for environment monitoring and food safety

Authors: Nyepudzai Charsline Gatsi[1]; Gugu Mhlongo[2]; Nosipho Moloto[3]; Rudolph Erasmus[3]; Martin Ntwaeaborwa[4]

[1] *University of the Witwatersrand, Johannesburg*

[2] *CSIR/UFS*

[3] *University of the Witwatersrand*

[4] *School of Physics, University of the Witwatersrand, Johannesburg.*

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The release of toxic gases from modern industries seriously threatens the environment and human safety [1,2]. Many researchers are therefore committed to developing inexpensive and effective sensors for detecting and monitoring such gases using semiconductor metal oxide (SMO) nanostructures [3]. In this work, a series of studies were conducted to investigate the gas sensing performance of unmodified and noble-metal-modified Ga2O3 nanorods prepared using a microwave-assisted hydrothermal method followed by heat treatment. Variation in the heat-treatment temperature induced controlled polymorphism, morphology, and structural defects in Ga2O3. The gas sensing measurements revealed a highly selective response, fast response (45s)/recovery (42s) times, and low detection limit of 0.61 ppm towards CO for the β-Ga2O3 sensor at a working temperature of 165 ℃. The β-Ga2O3 outperformed the α-Ga2O3 and α/β-Ga2O3 polymorphs due to more active surface sites offered by the high surface area and controlled donor and acceptor defects such as VGa and VO, respectively, for improved surface-target gas interaction. The decoration of β-Ga2O3 nanorods surfaces by 1mol% of noble-Ag nanoparticles demonstrated an optimum response coupled with a fast response/recovery time of 38/60 s towards ethylene gas at a lower working temperature of 140 ℃. DFT calculations and experimental characterizations revealed that high ethylene sensing benefited several factors including higher adsorption energy of ethylene compared to other target gases, sensitization and catalytic effects of surface plasmonic Ag metals, high surface area and high concentration of defects related to VO and VGa thus offering more active sites for surface-gas interaction. This work demonstrates the potential CO and ethylene sensing capabilities by unmodified β-Ga2O3 and 1mol%Ag-modified β-Ga2O3, respectively. Ethylene detection is important in food safety–quality monitoring and control in the fruit supply chains [4].

Keywords: Ga2O3; polymorphism; noble metals (Ag, Au); carbon monoxide; ethylene; gas sensing.

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Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics of Condensed Matter and Materials Track 1 / 136

Effect of Ruthenium dopant on the sensitivity of alpha iron oxide (α-Fe2O3) to Flammable and Hazardous Gases

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Co-authors: C.L Ndlangamandla C.L [2]; Nkosi Steven S [3]; Sunday A. Ogundipe [4]

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The increase in the number of manufacturing industries in the recent time has both positive and negative impact on our environment and the human health. The use of heavy duty machines in manufacturing industries causes the release of flammable and hazardous gases, which affect the human health, into the atmosphere. A lot of research efforts have been focused on the detection and monitoring of these gases using metal oxide semiconductor materials. This study investigates the gas sensing performance of Ruthenium-doped alpha iron oxide towards the flammable and hazardous gases. The alpha iron oxide doped with different weight percentage of Ruthenium were synthesized by co-precipitation method. The samples underwent some characterization techniques, such as X-ray diffractometry, thermogravimetric analysis, x-ray photoelectron spectroscopy, Brunauer-Emmett-Teller surface area analysis, scanning electron microscopy, and high resolution transmission electron microscopy, to study certain properties of the material. The sensors were fabricated by using the drop-casting method, and the sensors were tested for gas sensing performance, at 225 ^{0}C operating temperature, toward LPG, Ethanol, Propanol, Ammonium (NH3) and H2S. The pure sample (α-Fe2O3) was more sensitivity to the target gases with the response being 24.41 toward LPG, while the response decreased upon addition of ruthenium to alpha iron oxide. Ruthenium was found to be unsuitable as dopant material in alpha iron oxide for gas sensing application.
Keywords: Gas sensing, Dopant concentration, Alpha-Fe2O3-based sensor, Sensitivity, Flammable gases.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Nuclear, Particle and Radiation Physics / 138

Extraction of the Top Quark Yukawa Coupling

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Corresponding Author: j.mitchell@cern.ch

An exploration into machine-learning based optimisation techniques applied to the extraction of the top quark Yukawa coupling (Y_t) from top quark pair production in the dilepton final state, using proton collisions recorded by the ATLAS experiment in LHC run 2 and 3 is presented. Electroweak corrections for the exchange of the Higgs boson between the top quark and the top anti-quark for different values of Y_t result in changes to the kinematic distributions of the top quark and top anti-quark system close to the $t\bar{t}$ production energy threshold. The aim of this analysis is to use the kinematic distributions of the $t\bar{t}$ events in the dilepton final state to constrain the value for Y_t. The

observables that are most sensitive to Y_t are the invariant mass of the $t\bar{t}$ system, $m_{t\bar{t}}$, and the difference in rapidity, $\Delta y_{t\bar{t}}$. As the decay products of the $t\bar{t}$ system involve neutrinos in the dilepton final state, reconstructing the top quark and top anti-quark introduces resolution effects and additional systematic uncertainties. The proxy observables $m_{l\bar{l}b\bar{b}}$ (invariant mass of the $l\bar{l}b\bar{b}$ system) and Δy_{lblb} (the difference in rapidity between the two lb pairs) are used to mitigate this effect. In this talk, I will discuss the current state of the project, as well as future plans.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Applied Physics / 139

Development and testing of an external cavity diode laser and controller

Author: Kessie Govender[1]

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Diode lasers are compact, low-cost devices that are widely used in many applications requiring coherent light. However, for high precision atomic spectroscopy applications these devices are not suitable due to their large spectral linewidth. The laser wavelength is also dependent on the operating temperature and laser current. One way around the large linewidth problem is to enclose the diode in an external cavity arrangement as follows: the back facet of the diode is usually reflecting, and this can be used as one of the mirrors forming the cavity. The other mirror of the cavity can be a diffraction grating that is placed in front of the diode, directing one of orders of the diffracted light back into the diode. The diffraction grating is mounted on a piezo electric transducer, thus allowing fine control of the cavity length. This arrangement is referred to as an external cavity diode laser. Further, by using feedback control of the diode current, temperature and cavity length, the wavelength can be accurately controlled.
In the present project we have developed and tested a diode laser in an external cavity arrangement for applications in laser cooling of atoms and quantum optics experiments. The laser head consists of a diode laser and an external cavity using a diffraction grating as discussed above. The laser head also contains a piezo electric device for fine tuning of the cavity length, as well as a Peltier device for temperature control of the diode. The laser controller consists of feedback control circuits to adjust the diode current, the cavity length and the temperature of the diode. Also contained within the controller is a digital data acquisition module for monitoring system parameters and a PC interface. In this paper we will provide the performance characteristics of the system, including the temperature stability of the laser head, and linewidth measurements. Further, we have used the facility of controlling the temperature and current to study how the output wavelength varies with changes in operating temperature and current, and these results will also be presented.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Applied Physics / 140

Enhancing the photocurrent response of morphology tailored Cu2O nanostructures for photoelectrochemical water-splitting

Author: Mano Mosalakgotla[None]

Co-author: Mmantsae Diale

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Cuprous Oxide (Cu2O) nanostructures are known for their wide range of applications in photovoltaic devices, photoelectrochemical (PEC) cells, gas sensing devices and catalysts. They possess unique properties which are beneficial for PEC applications such as tunable narrow bandgaps and suitable band-edge positions. Furthermore, they are abundant and non-toxic in nature. Cu2O nanostructures such as nanospheres, nanocubes, nanorods, nanoflowers and nanowires have been previously achieved for effective PEC applications, respectively. In this study, we have fabricated Cu2O thin films prepared on fluorine-doped tin oxide (FTO) substrates. The morphology of the thin films was altered through the synthesis of various Cu2O shapes (nanotubes, nanosheets and nanodisks), particle sizes and annealing temperatures. The highly crystalline Cu2O nanostructures were confirmed by RAMAN spectroscopy. The surface morphology, chemical composition, and crystal structures of the prepared Cu2O thin films were investigated using the Field Emission Scanning Electron Microscope (FE-SEM) and Transmission Electron Microscope (TEM). The roughness of the surface was studied using an Atomic Force Microscopy (AFM). Ultraviolet–visible spectroscopy (UV-Vis) was used to study the photoabsorbance of the films. Lastly the thin films were used as photoelectrodes in a three-electrode electrochemical system to study their PEC properties. The enhanced photocurrent response of the films is attributed to the altered morphology, strong photoabsorbance, crystallization and low resistance of the transfer of charge carriers at the solid/liquid interface of the films. This study gave emphasis on the role of changing the morphology of Cu2O nanostructures to improve the process of water reduction on the photocathode/electrolyte interface.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Astrophysics & Space Science / 141

Galactic transients discovered in the MeerTRAP real-time, commensal single pulse search with MeerKAT

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MeerTRAP is a European Research Council funded search for fast radio transients with MeerKAT. The project uses a custom backend at the telescope that operates commensally with the MeerKAT Large Survey Projects (LSPs), collecting voltages from the antennas to form hundreds of beams on sky. These beams are continuously searched for millisecond-duration pulses from fast radio transients such as pulsars, magnetars, Rotating Radio Transients (RRATs) and Fast Radio Bursts (FRBs). In over three years of continuous operating we have amassed thousands of hours on-sky and discovered over 100 new radio transients. In this talk I give an overview of the dozens of transients we have discovered within the Galaxy, the follow-up science we have done on them, and their implications for the broader transient population.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / **142**

Incorporation of copper nanorods in organic solar cells

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Co-authors: Nolwazi Nombona [2]; Mmantsae Diale [2]

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In this study, the plasmonic effect of copper nanorods (Cu NRs) inside PTB7-Th:IEICO-4F to improve light scattering in organic solar cells have been investigated. Copper nitrate (CuNO3) is reduced with poly(vinylpyrrolidone) (PVP) in which the solution is heated in an autoclave to obtain Cu NRs. Cu NRs are deposited in PTB7-TH:IEICO-4F and spin coated on top of glass substrate followed by the blend poly(3-hexylthiophene): phenyl-C61-butyric acid methyl ester (P3HT: PCBM). The transmission electron microscopy (TEM) results show cylindrical shapes of Cu NRs with grain size of 50.3±0.5 nm. The UV-Vis spectroscopy revealed that NRs are absorbing in the visible range by showing plasmonic resonance at around 570 nm along with peaks of PTB7-TH:IEICO-4F, PCBM and P3HT at 950, 333 and 445 nm respectively. The X-ray diffraction (XRD) confirmed the FCC structure of Cu NRs with (111), (200), (220), and (310) phases in which the (111) peak was the most intense. Raman has also confirmed the existence of P3HT: PCBM, PTB7-TH:IEICO-4F and Cu NRs by showing the peaks of each structure. From this study, Cu NRs have a potential application in organic solar cells.
Keywords: Nanorods, solar cell, light scattering, PTB7-TH:IEICO-4F, P3HT:PCBM

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / **143**

POLARIS PEPT for Proton Beam Tracking

Authors: Alice Roux[None]; Steve Peterson[None]

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Proton therapy offers an advantage over traditional radiotherapy by depositing a therapeutic dose within a small volume. By exploring the secondary radiation from proton-nuclei interactions in the target, the energy deposition can be monitored to make up for the lack of {\it in vivo} dose measurements. One such method is Positron Emission Particle Tracking (PEPT) using PolarisJ Cadmium Zinc Telluride (CZT) detectors. PolarisJ detectors are chosen due to their high position sensitivity and have been shown to detect positron emitters to sub millimeter precision. By placing two Polaris

detectors face to face beside a target irradiated by a proton beam, the secondary 511 keV gamma ray pairs can be detected and identified. By applying a PEPT algorithm in the 2D plane perpendicular to the beam line, the position of the beam line is found as well as the positron production distribution within the target. This method can be used to evaluate the positron production along a 66MeV proton beam incident on water, HDPE and graphite targets. The positron production distribution from the proton beam is compared to Monte Carlo simulations predicting where along the beam line different β^+ reactions occur for the various target materials. As the position of these peaks occurs a fixed distance away from the Bragg Peak, the location of the dose deposition within the target can be located. The use of the PolarisJ detectors has the potential to improve the accuracy of dose measurements during proton therapy.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Theoretical and Computational Physics / 144

Quantum black holes and holography

Author: Sam van Leuven[1]

Co-author: Vishnu Jejjala

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It is often said that Einstein's theory of gravity (GR) and quantum field theory (QFT) are incompatible. I will present an argument for this claim based on thermodynamic properties of black holes in asymptotically flat spacetime. Applying similar reasoning in anti-de Sitter spacetime suggests that in this case the theory of gravity in D dimensions could be compatible with a quantum field theory, albeit one that lives in D-1 dimensions! This is a manifestation of the concept of holography, a promising route to a quantum theory of gravity. After a brief introduction to its realization in string theory, known as the AdS/CFT correspondence, I will discuss how this framework provides a quantum statistical framework to understand black hole entropy. Finally, I will discuss how recent work of me and my collaborators extends these successes in new directions. In our work, exciting new generalizations of modular forms play a key role.
The talk is aimed at a general audience and will assume only a basic familiarity with concepts in GR and QFT.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 2 / 145

Developing the Temperature Mapping Plugin of the Tile Calorimeter of the ATLAS Detector within Tile-in-One

Authors: Lungisani Sipho Phakathi[1]; Betty Kibirige[1]; Juraj Smiesko[2]; Sanele Scelo Gumede[1]; Filipe Martins[3]

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In order to continuously analyse the tile hadron calorimeter temperature data of the ATLAS off-line, the Tile-in-One (TiO) must be fully exploited. The Tile Calorimeter (TileCal) is a sampling hadronic calorimeter covering the central region of the ATLAS experiment, with steel as the absorber and plastic scintillators as the active medium. Wave Length Shifting fibres (WLS) gather light produced in each plastic scintillators. The WLS subsequently transmit that light into Photo Multipliers Tubes (PMTs). The TiO is a collection of small, independent web tools called plugins. Plugins assess the quality of data and conditions for ATLAS TileCal. The TiO web platform needs to be highly flexible and simple to maintain in order to be beneficial to plugin developers as well. An environment was created that allows users to use the Detector Control System (DCS) Data Viewer (DDV), to request temperature information from the DCS. This paper shows the successfulness of developing the temperature plugin and the mapping of it. The work aims to study the variation of temperature inside the drawers. Reason for this, is to know the stability of the electronics, and gain stability of the PMTs. Finding a simple way to display not only the state of one specific module but also the status of the entire detector is the main goal of the stable temperature plugin.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / **147**

Theory and Phenomenology of Relativistic Heavy-Ion Collisions

Author: Amogelang Moeng[1]

Co-authors: Siphe Somathube [2]; Mziwandile Sibiya [3]; Nkosikhona Gabela [3]; Vhahangwele Makumbane [4]; Dawit Worku [5]; Azwinndini Muronga [6]

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In high-energy physics, the study of the Theory and Phenomenology of Relativistic Heavy-Ion Collisions examines how atomic nuclei behave when they collide at exceedingly fast speeds, nearly at the speed of light. These collisions produce rich observable signatures that can provide insight into the properties of quark-gluon plasmas (QGPs), a state of matter believed to exist at high temperatures and densities. This study will focus on understanding the various stages of Relativistic Heavy-Ion Collisions (RHIC), as well as the signatures associated with some of the stages. One of

the key signatures of QGP formation is the suppression of J/ mesons, the bound states of charmed and anti-charmed quarks. This suppression is based on the strong forces between quarks and anti-quarks being screened by the hot and dense medium produced by the collisions. The degree of J/ suppression can provide information about the temperature and density of the QGP. The increase in strangeness production is another key indicator of QGP formation. Strangeness is a characteristic of a few subatomic particles, including the strange quark, and it is not preserved in strong interactions. In QGP, the presence of many strange quarks and antiquarks is thought to increase the abundance of strange particles.

Overall, the research on these signatures of heavy ion collisions sheds light and provides important insights into the properties of QGPs and how matter behaves in extreme conditions. Furthermore, the study will review on how recent high energy heavy ion experiments at RHIC and LHC are consistent with the production of the quark gluon plasma in high energy Pb+Pb collisions.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / 148

Effects of defects on gas sensor performance of β-Ga2O3

Authors: Nyepudzai Charsline Gatsi[1]; Gugu Mhlongo[2]; Nosipho Moloto[3]; Rudolph Erasmus[3]; Martin Ntwaeaborwa[1]

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The gas sensing performance of a material partly depends on its defect property, especially the oxygen vacancy (VO) content [1]. The trace amounts of common impurities such as Cr3+ and N in Ga2O3 nanostructures significantly influence their defect-emission profiles [2,3]. In this work, we investigated the effect of unintentionally doped Cr3+ and N defects in conjunction with the intrinsic donor (VO) and acceptor (VGa) defects on the gas sensing performance of β-Ga2O3 nanorods. The photoluminescence and gas sensing results demonstrate a significant influence on the response/recovery times from the unintentionally doped Cr3+ and N defects in β-Ga2O3. Fast response times are key in rapid detection of toxic gases such as CO and quick recovery is important for reusability of the sensing material.

Keywords: Ga2O3; intrinsic defects; oxygen/gallium vacancies; gas sensing.

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Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics of Condensed Matter and Materials Track 1 / 149

A machine learning approach to prediction of bandgap and optimum efficiency of perovskite solar cells based on SCAPS 1-D data simulation

Author: Dakalo Rollet Mashamba[1]

Co-authors: Mandla Msimanga [1]; Abraham Dimitri Kapimkenfack [2]

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Abstract

Recent advances in perovskite solar cells (PSCs) have yielded power conversion efficiency (PCE) values exceeding 25.5% within a decade from their inception. Despite this rapid growth in PCE, one of the major drawbacks hindering large scale commercialization of PSCs is the toxicity of the lead (Pb) component in their composition [1]. Partially or wholly substituting Pb with other environmentally friendly metal elements offers a solution to circumvent this challenge. Due to the vast chemical landscape of perovskite materials, composition selection for mixed perovskites is still largely through tedious, costly and labour-intensive trial and error experiments [2].

In this contribution, solar cell capacitance simulator (SCAPS) was utilized to simulate a PSC device of methylammonium tin/lead iodide ($MASn_xPb_{1-x}I_3$). The simulated open voltage circuit (V_{OC}), fill factor (FF), current density (J_{SC}) and efficiency of the solar cell were optimized by varying input parameters of the perovskite absorber layer: thickness (200 – 1500 nm) and the bandgap (1.18 – 1.6 eV) corresponding to Sn_xPb_{1-x} composition. A set of supervised machine learning (ML) models were trained to predict the relative effect of varying the composition on the bandgap. Based on SCAPS simulated data, a second ML model was designed to predict the best possible PCE using the predicted bandgap and layer thickness values as input parameters. The results suggest that ML in conjunction with numerical SCAPS simulations can be an effective approach to accelerate discovery [3] of efficient, low cost and less toxic PSCs through narrowing down possible perovskite combinations to just a few permutations.

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Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / 150

ROLE OF NUCLEAR INTERACTIONS ON THE GROUND-STATE STRUCTURE OF HELIUM-6 THREE-BODY SYSTEM

Authors: Mahabe Mahatikele[1]; Bahati Mukeru[1]; Gaotsiwe Rampho[1]

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In the study of three-body weakly-bound systems, a three-body interaction is always introduced to take care of the dynamics that cannot be accounted for by two-body interactions. In order to get some insight into these dynamics, in this presentation, we study the relevance of the three-body interaction as the number of neutrons in the three-body system increases, considering helium-6. It is found that by removing this interaction from the structure of the system, the ground-state binding energy of the helium-6 system drops by approximately 80%. This shows that the three-body interaction plays a significant role in the dynamics of a three-body weakly-bound neutron-rich system.

Keywords: Three-body system, Three-body interaction, Binding energy.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics of Condensed Matter and Materials Track 1 / 151

Single crystal growth and physical properties of tetragonal $BaMn_2P_2$

Authors: Bincy Susan Jacobs[1]; Abhishek Pandey[2]

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The discovery of unconventional superconductivity (SC) in doped iron-based arsenide $BaFe_2As_2$ [1] crystallizing in $ThCr_2Si_2$-type structure ignited interest in 122 tetragonal systems. Substituting iron with other $3d$ or $4d$ transition metal ions that constitute the metal-pnictide sublattice in similar systems have yielded interesting results including, but not limited to, low-temperature SC [2], half-metallic behaviour [3], new layered magnetic phases [4] and highly frustrated itinerant magnetism [5]. The Mn based $BaMn_2Pn_2$ compounds [Pn = P, As, Sb, Bi] are small band gap semiconductors with stacked-square-lattice of Mn ions that order antiferromagnetically at temperatures higher than room temperature. Although As, Sb and Bi based compounds have been thoroughly investigated [6-9], the experimental work on $BaMn_2P_2$ is dated and limited [10,11]. In this contribution, we report the synthesis and growth of single crystals of $BaMn_2P_2$ as well as its structural, electronic, magnetic and thermal properties. Electrical resistivity and heat capacity measurements indicate that $BaMn_2P_2$ has an insulating ground state with a small band gap. Anisotropic magnetic susceptibility

measurements show that similar to its As-, Sb- and Bi- counterparts, $BaMn_2P_2$ has collinear Néel type antiferromagnetism below T_N = 795(15) K, which is the highest value for 122- pnictide compounds reported so far. The magnetic susceptibility increases above T_N suggesting that antiferromagnetic correlations persist above the magnetic ordering temperature—a feature which was also observed in the As-, Sb- and Bi- based compounds. This can be explored further through hole-doping studies as in the case of $BaMn_2As_2$ with T_N = 618 K, which resulted in half-metallic behaviour with T_c = 100 K which is of significance as high T_c half-metals are ideal for spin-polarized transport-based applications. These results were recently published in Phys. Rev. Mater. **7**, 044410 (2023).

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No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Nuclear, Particle and Radiation Physics / 152

Probing clustering in light nuclei through particle decay measurements

Authors: Retief Neveling[1]; Philip Adsley[2]; Kevin Li[3]; Lindsay Donaldson[4]; Armand Bahini[5]; Luna Pellegri[6]; J.W. Brummer[1]; SANDILE JONGILE[1]; Mathis Wiedeking[1]

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The concept of clustering - that nuclei can contain sub-groups of correlated nucleons combining into larger structures rather than consisting simply of individual nucleons - has become extremely important in understanding the structure of light nuclei. The Hoyle state, the second 0+ state at 7.654 MeV in 12C, is considered the archetype of alpha cluster states in nuclei, and its existence is considered to be closely tied to that of organic life, as it is the portal through which 12C is created in stars. While this state has been, and remains, the focus of numerous theoretical and experimental studies, some of which were performed at iThemba LABS, the search for analogues of the Hoyle state in the neighboring A=11 and A=13 nuclei is also of interest. We will focus on the A=13 system, and in particular on 13N, which can be populated through a (3He,t) reaction. The utility of particle decay measurements from excited states in 13N in search of odd Hoyle states will be discussed.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Photonics / **153**

Optical Tweezers Towards Single-Cell Analysis

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Optical Tweezers have become a popular tool for manipulating micron diameter particles with minimal influence on the properties of said particles. By using a single laser and a high numerical aperture lens, these particles can easily be confined and moved for the researcher's purpose. Such manipulation allows for the measurement of piconewton forces, which makes it possible to measure the molecular forces inside biological cells and to characterise fluid dynamic systems in terms of flow rate and shear forces. These capabilities have led to significant contributions to the fields of biochemistry and biomedicine. Another groundbreaking tool for studies in these fields are microfluidic "lab-on-a-chip" devices.

By combining the manipulation capabilities of Optical Tweezers with a microfluidic device's ability to control the external environment of cell, the response of the cell to external stimuli can be measured. This includes monitoring drug uptake as a function concentration, as well as the expression of various biomolecules on a single-cellular level. The microfluidic device allows for maximal control and change of the extracellular environment while the optical tweezers create an easy method of moving single cells to these controlled environments. This process can be parallelised which can lead to the high throughput analysis of therapeutic drugs. This integrated system will also have the benefit of providing a sterile environment to do biochemical studies in but also ensures minimal influence from unwanted external factors.

In this talk, we will discuss the principle behind single-beam Optical Tweezers and the construction of such a setup and under what conditions a stable trapping is achieved. This setup includes custom fluorescence- and Raman spectroscopy modules to the setup as well as a force calibration module which allow for the characterization of the trap. The system can be further expanded with the inclusion of a spatial light modulator to speed up analysis and increase throughput. Furthermore, we look at the basic operating principle of microfluidic devices and different designs of these devices. We then look towards biological analysis of yeast strain saccharomyces cerevisiae, known more commonly as brewer's yeast, and the conditions which allow for such cells to be trapped. Initial proof of principle measurement will be shown. .

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Applied Physics / 154

Comparative Analysis of Numerical Methods for Assessing Wind Potential in Fort Beaufort, South Africa, using Two-Parameter Weibull Distribution Model.

Author: Ngwarai shambira[1]

Co-authors: Golden Makaka [2]; Patrick Mukumba [1]; Chipo Shonhiwa [2]

[1] *University of Fort Hare*

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The utilisation of wind energy has the potential to both alleviate South Africa's energy crisis and increase access to electricity in remote areas that lack connections to the national grid. Wind energy is a clean, abundant, and inexhaustible renewable energy source that can effectively reduce carbon dioxide emissions and mitigate the adverse effects of climate change that South Africa and its neighbouring countries are experiencing. This is usually in the form of heat waves and cyclones. South Africa has significant potential for wind energy generation, especially in coastal regions of the Eastern Cape Province. To determine the wind characteristics and wind potential of an area, an accurate wind distribution model is essential. Therefore, this study examines eight numerical methods for estimating the Weibull parameters to obtain a suitable model. Five and half years (January 2015–July 2020) hourly averaged wind data collected at an anemometer height of 10 m at Fort Beaufort weather station was used. The two-parameter Weibull distribution was used to fit with the wind data. In addition, eight distinct numerical algorithms were utilised to calculate the Weibull shape (k) and scale (c) parameters for the distribution, namely, the mean, standard deviation method (Msdm), method of multi-objective moment (MofMoM), probability-weighted moments based on power density method (PwmbpdM), WAsP method (WM), method of mabchour (momab), openwind method (Owm), energy pattern factor method (Epfm), novel energy pattern factor method (Nepfm). A goodness of fit test was carried out to evaluate the performance of each algorithm, and their results were analysed based on six statistical error indicators: mean absolute bias error (MaBE), root mean square error (RMSE), wind power density error (WPDE), Kolmogorov-Smirnov (KS) test, Anderson-Darling (AD) test, and chi-squared statistical test. The results showed that the openwind method was the best algorithm and gave Weibull shape (k) and scale (c) values of 1.67905 and 3.35800, respectively. The value of the predicted wind power density of the Fort Beaufort area was 38.45 W/m2. This value revealed that only small-scale wind power generation projects should be utilised in this area for lightning, battery charging, or water pumping using small-scale wind turbines. It is recommended to use augmentation systems such as concentrators, diffusers, and invelox to shroud the wind turbines and lower the cut-in wind speeds, as most turbines available on the market require wind speeds above 5 m/s to start operating in this area. The findings also revealed that the prevailing wind direction in the Fort Beaufort area is mainly from the southeast (SE).

Keywords: Weibull distribution; wind power density,South Africa, renewable energy, Wind energy, wind speed

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Consent on use of personal information: Abstract Submission:

Photonics / 155

Solution phase photodegradation studies of PCDTBT

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Co-author: Gurthwin Bosman [1]

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Poly[N-9′-heptadecanyl-2,7-carbazole-alt-5,5-(4′,7′-di-2-thienyl-2′,1′,3′-benzothiadiazole)], PCDTBT, is a conjugated donor polymer used in low bandgap organic solar cells (OSCs). OSC efficiencies decrease when exposed to light, oxygen, or water. The effects of various excessive light conditions on degrading dilute PCDTBT in solution are investigated in this work. A custom photodegradation fluorescence spectrometer setup was constructed to rapidly photodegrade PCDTBT solutions with a chosen laser intensity and wavelength. Changes in the recorded fluorescence spectra reflect structural polymeric changes induced by the high intensity laser irradiation. This, combined with the steady state absorption profile before and after 3 hours of continuous photodegradation, confirms that chain scission (bond breaking) occurs. Extracted fluorescence intensity decay rates suggest rapid initial degradation within the first 30 minutes followed by a much slower degradation regime. Other structural information is also gained, including chain length distributions and the degree to which conformational rearrangement of the polymer backbone plays a role during degradation. These findings indicate that this type of constructed laser fluorescence spectrometer setup is a valuable spectroscopic tool which could be of use to the OSC community for studying photodegradation dynamics. Importantly it allows for isolating and comparing the effects of different excitation intensities and wavelengths on photodegradation which cannot be straightforwardly done with currently ubiquitous broadband solar simulators.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / 156

First principle study of structural and thermodynamic stability of ternary NaVSe2

Author: DAVID TSHWANE[1]

Co-authors: Lethabo Mogakane [1]; Prettier Morongoa Maleka [1]; Rapela Maphanga [2]; Ratshilumela Steve Dima [3]

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Ternary AIIBIVCVII structures have received a great deal of attention from both technological and scientific perspectives due to their optoelectronic properties and both p- and n-type electronic conductivity. Among them, NaVSe2 dichalcogenide compound promises excellent intercalation and high conductivity. However, details on the structural, and electronic properties of NaVSe2 remain limited, especially at the atomistic scale. The present study employed density functional theory approach using different functionals such as GGA-PBE, GGA-PBEsol, and LDA to investigate the structural, thermal, and electronic stability of NaVSe2. The results showed that the ΔHf <0 for NaVSe2, which implies that the phase is thermodynamically stable. In addition, it was found that GGA-PBE

functional is the most suitable function than GGA-PBEsol and LDA functional. Moreover, the partial density of state was computed wherein Se 4p states contribute mainly to the valance band whilst the conduction band mainly consists of V s- and Se -p states.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 2 / 157

Investigation of the novel tetragonal compounds BaT_2P$_2$(T = Co, Ru, Pd)

Authors: Arthur Van der Spuy[1]; Bincy Susan Jacobs[2]; Abhishek Pandey[3]

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[2] *University Of Johannesburg*

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Tetragonal ACo$_2Pn_2$ (A: alkali or alkaline earth metals, Pn: pnictides) compounds are known for their exotic structure-property relationships [1-4]. Some of these compounds have also been reported to exhibit unusual behaviors, like the recently observed positive curvature in electrical resistivity of highly pure single crystals of KCo$_2As_2$ [5]. In the present work, we investigate the structural, magnetic, transport and thermal properties of polycrystalline samples of unexplored materials BaT_2P$_2$ (T =Co, Ru, Pd). Our study confirms that BaCo$_2$P$_2$ and BaRu$_2$P$_2$ crystallize with ThCr$_2$Si$_2$-type tetragonal structures while BaPd$_2$P$_2$ crystallizes with a CeMn$_2$Si$_2$-type tetragonal structure. All three compounds show metallic behavior and sizable density of states of conduction carriers at the Fermi level and do not exhibit any phase transition down to the lowest temperature of our measurements. We attempt to model the physical properties data of these compounds as well as explore the effect of lowering the crystal symmetry, if any. The experimental results will be discussed in detail and compared with the existing literature.

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Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / 158

Performance Operation of a Greenhouse Biogas Digester

Authors: Mandilakhe Mzobotshe[1]; Patrick Mukumba[None]; Stephen Tangwe[None]

[1] *University of Fort Hare*

Corresponding Author: 201716588@ufh.ac.za

South Africa is faced with an energy crisis as it relies more on energy from fossil fuels. The use of Renewable energy technologies can be a solution to current energy crisis in South Africa leading to continuous load shedding. Waste-to-energy conversion is playing a significant role in advancing economic development and health quality in society. One of the technologies that exploit waste-to-energy conversion is biomass technology. Renewable energy biogas from biomass can be used for electricity generation, heating, lighting purposes and fuel for vehicles. For optimum biogas production, solar energy can be used to provide suitable digester temperatures. In this research, a portable plastic biogas digester housed inside a greenhouse cavity was assembled and fed with cow dung. The pH, ambient temperature, slurry temperature, and temperature inside the greenhouse cavity measured taken daily. The biogas yield was measured by the serial residential (SR) diaphragm biogas flow meter, and the methane composition was measured with the use of the SAZQ biogas analyser. The influence of temperature on biogas fermentation was investigated in the study. A heat transfer model of biogas fermentation was built based on the project and as a result the influence of temperature on biogas fermentation was investigated in the study. The results depicted that the gas production rate of biogas fermentation increases with the increase of temperature within a certain range, and the maximum biogas production occurred when the pH was in the range of 6.84 to 7.03. The methane composition of the biogas was above 50%. it was observed that a digester housed inside a greenhouse envelope can keep the slurry temperature in the optimal mesophilic temperature range of 34oC –36oC, which is ideal for anaerobic digestion.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics of Condensed Matter and Materials Track 1 / 159

Deposition time-dependent properties of electrodeposited CdSe thin films from cadmium nitrate source for energy harvesting application.

Author: Ahmed Yimamu[1]

Co-authors: F.B Dejene [2]; O.K Echendu [3]; J.J Terblans [1]; H.C Swart [1]; S.J Motloung1 [1]

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[2] *WSU*

[3] *Federal University of Technology*

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Electrodeposition of CdSe thin films using a two-electrode configuration was performed at different deposition periods such as 5, 10, 15, 20, and 30 min on conductive glass substrate fluorine-doped tine oxide (FTO). Structural, optical, electrical, surface morphology, surface roughness, and elemental composition of CdSe thin films for both as-deposited and annealed samples were investigated by using X-ray diffraction (XRD), UV–VIS spectrophotometry, Photoelectrochemical cell analysis (PEC),

scanning electron microscopy (SEM), scanning probe microscopy (SPM) and energy-dispersive X-ray spectroscopy (EDS) respectively. The structural properties show that CdSe thin films are found in cubic and hexagonal structures. Optical properties analysis shows that CdSe thin film absorbance increased with deposition time. The energy band gap varied between 1.69 and 1.85 eV for both as-deposited and annealed samples. PEC measurement confirmed that both as-deposited and annealed samples are n-type conductivity. The surface morphology analysis shows that the film covered the glass substrate, and the shape, grain size, and morphology changed with deposition time. The scanning roughness analysis confirmed that the average surface roughness was recorded as-deposited films 35.72, 53.61, and 45.45 nm for annealed samples 49.18, 55.26, 45.9 nm with deposition times 5, 20, and 30 min, respectively. The elemental composition analysis confirmed that both Cd and Se were present in the film, and their percentage composition varied with deposition time. In thin film solar cell devices, the thickness plays a great role and is controlled by deposition time. The CdSe film deposited at a short time of 5 min has potential application for the window (buffer) layer, and for a longer time, 30 min, is used as an absorber layer for solar cell devices.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / 160

Geant4 simulation for detector development and PET imaging

Author: Busani Bhengu[1]

[1] *Student*

Corresponding Author: bhengub@live.com

The main aim of this project will be to perform GEANT4 simulation as part of the medical imaging project which will be done using the Modern African Detector Laboratory (MANDELA) at University of Zululand. The university of Zululand Physics department is collaborating with the university of York Physics department and the university of the Western Cape in this research. Through this research the Watts et al., have identified a number of potential benefits by using QE in PET. Part of this project is to investigate some of these benefits. Positron Emission Tomography (PET) is a nuclear medicine imaging technique used for medical research and for imaging of cellular and anatomical processes, and medical diagnosis. This imaging technique is based on two gamma photons produce by the annihilation of positron-electron pair. These two gamma photons of at least 0.511 MeV are predicted to the entangled. Gean4 simulations is an important tool used to investigate the predicted entanglement. Recently, research predicts that the PET scanners based on quantum entanglement will be more economically and sensitive than the present technology. PET has been in existence since the 1970s due in large part to the pioneering work of Michael Phelps, PhD, Michel Ter-Pogossian, PhD, and others in the fields of medical physics and nuclear medicine. Through detailed experiments and simulations, the benefits of take advantage of the quantum entanglement of linear polarization between the two positron annihilation photons utilized in PET will be investigated. Implementing Geant4 simulation, which have included the predicted influence of quantum entanglement is confirmed by comparison with experimental data from a PET demonstrator apparatus. The development of quantum-entangled PET provides fresh approaches to major problems in next-generation imaging. We describe a straightforward technique to measure and eliminate in-patient dispersion and random backgrounds using only the quantum entanglement information in the PET events as an example of the potential advantages.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc. Physics

Poster Session 2 / **161**

Development of a nonlinear response surface model to predict the volume of biogas yield of a fixed dome digester charged with cow manure

Authors: Mandilakhe Mzobotshe[None]; Patrick Mukumba[None]; Stephen Tangwe[None]

Corresponding Author: 201716588@ufh.ac.za

Waste to energy conversion is playing significant role in advancing economic development and health quality in the society. One of the technologies that exploits waste to energy conversion is biomass technology. The study focused on the development of a response surface model to predict the biogas production with input parameters being pH of slurry, slurry temperature and product of ambient temperature and global irradiance for an underground fixed dome digester fed with cow dung using continuous method. The fixed dome digester was fabricated with high density polyethylene (HDPE) PVC plastic and the data acquisition system comprised of temperature sensors, pH sensor, pyranometer, biogas analyser, gas flow meter and dataloggers. The results depicted that the hydraulic retention period for the anaerobic digestion was 50 days and the cumulative volume of biogas produced was 39.55 m3 while the reactor volume was 2.5 m3. It was determined that the measured daily biogas yield and the predicted value during the hydraulic retention period mimic each other with a correlation coefficient of 0.987 and a mean absolute error of 0.0002. The findings from the study can lead to the conclusion that the nonlinear surface response model can predict the biogas yield with high accuracy based on the acceptable values of the correlation coefficient and mean absolute error.

Keywords: fixed dome biodigester, waste-to-energy conversion, response surface model, correlation coefficient, mean absolute error

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Theoretical and Computational Physics / **162**

Wigner function approach to the classical limit of quantum Brownian motion and to the derivation of open quantum Brownian motion

Author: Ayanda Zungu[1]

Co-authors: Ilya Sinayskiy [2]; Francesco Petruccione [3]

[1] *Department of Physics, North-West University, Mafikeng Campus*

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Open quantum Brownian motion (OQBM) represents a new type of Brownian motion with an additional quantum internal degree of freedom. This framework was introduced by Bauer, Bernard, and Tilloy [1] as a scaling limit of discrete-time open quantum walks [2,3]. Sinayskiy and Petruccione (SP) have shown that OQBM can be derived from the microscopic Hamiltonian of the system, bath, and system bath interaction [4,5]. In this contribution, we report on the generalization of SP work. In our model, the inner degree of freedom is given by a two-level system, and the position operator describes the external degree of freedom. We derive the QBM master equation and use the Wigner function approach to perform the classical limit to obtain OQBM.

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Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 1 / **163**

Structural, Electronic, Mechanical and Thermodynamic Properties of Ternary NaVS2: DFT Study

Author: LETHABO MOGAKANE[None]

Co-authors: Ratshilumela Steve Dima [1]; Prettier Morongoa Maleka [2]; DAVID TSHWANE [3]; Rapela Maphanga [4]

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Structural, Electronic, Mechanical and Thermodynamic Properties of Ternary NaVS2: DFT Study
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2National Institute for Theoretical and Computational Sciences (NITheCS), Gauteng 2000, South Africa

Abstract:
Sodium-ion batteries have recently gained a lot of attention because they are environmentally benign and less expensive. The impact of Na atom deintercalation on olivine NaVS2 was examined for potential usage as a cathode material in Na-ion batteries. In this study, first-principle approach was employed to investigate ternary NaVS2 using plane wave pseudopotential method with different exchange correlation functions, GGA-PBE, GGA-PBEsol and LDA. Results revealed that trigonal NaVS2 phase are thermodynamical stable with $\Delta Hf < 0$. Optimized lattice parameters computed with GGA-PBE functional was found to be in good agreement with previous results. Furthermore, the partial density of states and the Mulliken population analysis were investigated to understand electronic properties and the effect of deintercalation on NaVS2 phases. In addition, the elastic properties were calculated to measure the mechanical stability of the structures.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 2 / **164**

FERMI ENERGY PREDICTION OF SODIUM-ION BATTERY CATHODE MATERIALS: A MACHINE LEARNING REGRESSION APPROACH

Author: Keletso Monareng[1]

Co-authors: Rapela Maphanga [2]; Petros Ntoahae [3]

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Abstract
Transitioning from fossil fuels to renewable energy sources is a critical global challenge, it demands advances at the materials, devices for the efficient storage and management of renewable energy. Energy researchers have begun to incorporate machine learning techniques to accelerate these advances. In this perspective, machine learning regression techniques are applied to a large amount of data to develop machine learning models that predict the Fermi energy of sodium-ion battery (SIB) cathode materials accurately. Thus, the importance of feature vectors were evaluated based on the properties of the chemical compounds and the elemental properties of materials constituents, with the estimated FCC lattice parameter, the average electronegativity, and the average density proving to be the most significant descriptors to predict Fermi energy. Based on the evaluation of various models, the light gradient boosting machine model was found to be the most accurate at predicting the fermi energy, with coefficient of determination and mean square error of 0.82 and 0.52 eV, respectively.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / **165**

First principles study of structural, elastic, electronic and optical properties of triclinic CsAlS2 chalcogenide.

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Abstract
The structural, elastic, electronic and optical properties of triclinic model CsAlS2 are investigated using the plane wave ultrasoft pseudopotentials approximation in the framework of density functional theory as implemented in CASTEP code of Material Studio package. The exchange correlation potential is treated with the generalized gradient approximation within the scheme of Perdew-Burke-Ernzerhof. The ground state properties are determined and the calculated elastic constant show that the CsAlS2 structure obeys the triclinic criterion. The obtained band structure and density of states predict the material to be an insulator with a direct band gap of 3.246 eV at 0 GPa. The optical properties are obtained and discussed, including reflectivity and absorption coefficient, which provide useful information for the future application of CsAlS2 in photovoltaics.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics of Condensed Matter and Materials Track 2 / 166

Effect of pressure on structural, mechanical, electronic and optical properties of LiAlS2, NaAlS2 and KAlS2 chalcogenides: A density functional theory study

Author: Boitemogelo Phale[1]

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3National Institute for Theoretical and Computational Sciences, NITheCS, Gauteng, 2000

Abstract
The structural, mechanical, electronic and optical properties of LiAlS2, NaAlS2 and KAlS2 chalcogenides are investigated by utilizing Perdew-Berke-Ernzerhof functional within generalized gradient

approximation under the context of density functional theory as a function of pressure. The mechanical properties are obtained using the Vight-Reuss-Hill approximation. The pressure dependent band structures and density of states are obtained using geometry optimization method. The calculated electronic density of states predict the insulating nature while the band structures exhibit the direct band gaps of 4.21, 3.70 and 3.62 eV for the triclinic LiAlS2, NaAlS2 and KAlS2 respectively, at 0 GPa. The optical properties including the absorption coefficient, refractive index and reflectivity are calculated and analyzed. Furthermore, the spectra of reflectivity curves are high in the ultraviolet regions suggesting they could be used as coating materials to avoid solar heating.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / **168**

Optimization of deposition voltage for growth of CdZrS thin films for window layer of CdTe-based solar cell device application.

Author: TSHEPO KARABO WILLIAM MOHAPI[1]

Co-authors: A.U. Yimamu [2]; K.G. Tshabalala [2]; S.J. Motloung [2]

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CdZrS thin films were synthesized by the two-electrode electrodeposition method at different growth voltages (1535-1570) mV with intervals of 5 mV on conductive glass substrate fluorine-doped thin oxide (FTO). Structural, optical, electrical, surface morphology, surface roughness, and elemental composition of the as-prepared and annealed CdZrS thin films were investigated by using X-ray diffraction (XRD), UV-vis spectrophotometry, photoelectrochemical cell analysis (PEC), scanning electron microscopy (SEM), scanning probe microscopy (SPM) and energy-dispersive X-ray spectroscopy (EDS) respectively. The structural characteristics revealed that the films have cubic and hexagonal mixed phases. Their energy band gap was found to change with the deposition voltage. PEC analysis verified that both the as-deposited and the annealed samples are p- and n-type conductivity. The surface morphology and roughness study demonstrates that the film completely covered the glass substrate and that the form, grain size, and morphology all altered with deposition cathode voltage. The elemental composition analysis confirmed the presence of Cd, Zr, and S in the films, and their percentage composition varied with deposition voltage. The overall analysis shows the addition of Zr in CdS thin films increased the band gap, and therefore, the prepared materials have potential application in p-n junction solar cells as a window (buffer) layer.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Photonics / **169**

Evaluation of Anticancer Effect of Punica granatum Extract in Combination of Hypericin Mediated Phototoxicity on MCF-7 Cells

Author: Nosipho Fakudze[1]

Co-authors: Paromita Sarbadhikary [1]; Blassan George [1]; Heidi Abrahamse [1]

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Cancer has been established as one of the prevalent causes of death globally, rating second after cardiovascular disease. The GLOBOCAN 2020 report has estimated global new cancer cases of approximately 19.3 million, with a death toll of nearly 10.0 million. The report also estimates about 2.3 million of new cases of female breast malignancy, making it the most commonly diagnosed cancer type. The 2020 South African National Cancer Registry recorded a 23.25% female breast cancer incident rate as the leading type of cancer. Natural plants and fruits have been important to the medical community due to their therapeutic properties and low cost. They contain phytochemicals important in cancer prevention and treatment. Punica granatum is a fruit with anticancer, antiproliferation, and antioxidant qualities. Its limitations come with its lack of water solubility and bioavailability. In recent years, combination therapy has gained interest among researchers and clinicians as one of the anticancer strategies to overcome the limitations of each modality to enhance the effective treatment outcome. Photodynamic therapy (PDT) is a photochemical based therapeutic modality that depends light excitation of photosensitizer to generate toxic reactive oxygen species to kill cancer cells. Hypericin is a natural photosensitizer with significant antitumor effects by targeting specific signaling pathways. Thus, this study aims to investigate the combined anticancer effect of P. granatum extract in combination with hypericin as a photosensitizer against breast cancer cells. MCF-7 treated with different concentrations (50-400 µg/ml) of P. granatum chloroform extract followed by 600nm of laser irradiation at IC50 concentration of hypericin with 5 J/cm2 light dose with. Post treatment cell variability was analysed by MTT assay, and morphological changes were visualized using brightfield microscopy and cell viability by live dead assay. Results have shown significant cytotoxic effects in combination therapy compared to single treatment alone. This study provides a promising approach to effective combination anti-cancer therapy using natural plant-based compounds.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Nuclear, Particle and Radiation Physics / 170

Discrepancies between (p,p') and (g,xn) experiments

Author: Lindsay Donaldson[1]

Co-authors: Philip Adsley [2]; Armand Bahini [3]; Johan Wiggert Brummer [1]; John Carter [4]; Sandile Jongile [5]; Retief Neveling [6]; Luna Pellegri [7]; Iyabo Usman [8]

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[5] *iThemba Laboratory for Accelerator Based Science*

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High energy-resolution proton inelastic scattering experiments with E_p = 200 MeV were performed on the even-even Nd isotope chain and ¹⁵²Sm. The experiments focussed on the excitation-energy region of the Isovector Giant Dipole Resonance (IVGDR) and made use of the zero-degree mode of the K600 magnetic spectrometer at iThemba LABS. A goal of the highlighted study was to confirm the *K*-splitting observed in previous photo-absorption measurements at Saclay. The comparison of the shape of the IVGDR in the transition from spherical to deformed nuclei yielded significant discrepancies between equivalent photo-absorption cross sections obtained from the K600 data and the photo-absorption data obtained at Saclay. In addition, discrepancies have also been observed between photo-absorption data taken at the Saclay and Livermore laboratories. These discrepancies will be discussed along with future investigations into the possible reasons for them, which include coincident particle detection experiments to study the (g,p) contribution to the overall cross section.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 1 / 171

The effect of acids precipitants on the synthesis of WO3 hierarchical nanostructures for highly selective and sensitive H2S detection

Authors: Thokozani Mpanza[1]; Ceboliyazakha Ndlangamandla[1]

[1] *University of Zululand*

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The detection and monitoring of H2S gas at high and lower concentrations is very crucial since this gas is highly toxic and can affect tissues and organs, especially in occupational environment. This work reports on the synthesis of WO3 nanostructures-based sensors for highly sensitive and selective H2S detection at low operating temperatures. These WO3 nanostructures were synthesized using pressurized hydrothermal process. Different acids from weak to strong (HNO3, H2SO4, and HCl) were employed as precipitants to form supposedly hierarchical and cube-like nanostructures of WO3. These WO3 nanostructures were characterized by XRD, SEM, TEM, XPS and BET analysis. The fabricated WO3 sensors were exposed to different target gases (CO2, H2, CH4, NH3, LPG and H2S) at different concentrations. They were found to be selective to H2S, and the WO3 precipitated by HCl otherwise referred to as WO3-HCl was found to be highly sensitive, with high response of S = 1394.04 towards 150 ppm of H2S at 125℃ operating temperature. The WO3 precipitated by H2SO4 named WO3-H2SO4 showed a high response of 141.64 at 125℃ operating temperature. Lastly, WO3 precipitated by HNO3 called WO3-HNO3, recorded a H2S response of 125.75 also at 125℃ operating temperature. The HCl-precipitated WO3 is a promising candidate for selective detection of H2S, being the most sensitive in the series.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Applied Physics / 172

Assessment of CO2 emissions in the rural set-up of the Vuwani area in Limpopo, South Africa.

Author: Lufuno Takalani[1]

Co-authors: Humbelani Thenga [2]; Sophie Mulaudzi [1]; Nnditshedzeni Eric Maluta [1]

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Abstract

The world is currently battling climate change through various mitigation and adaptation measures. Some of these measures include reducing greenhouse gas emissions, transitioning to renewable energy sources, implementing sustainable agriculture and forestry practices, and enhancing climate resilience in vulnerable communities. The Vuwani area plays a significant role in carbon emissions, where agriculture and land use change are major drivers of emissions. This area often has high levels of deforestation, burning of fossil fuels, and use of traditional biomass for cooking and heating, which contribute to carbon emissions. The assessment of CO2 emissions in the Vuwani area is a growing concern due to its potential impact on climate change. This study focuses on the rural area of Vuwani in Limpopo, South Africa, where CO2 emissions are high due to various anthropogenic activities. However, there was a gap in knowledge regarding the magnitude and sources of CO2 emissions in this area. The availability of data on CO2 emissions from the Vuwani eddy covariance flux tower filled that gap and shows the area as a source of carbon which can assist the country in formulating effective policies to mitigate climate change. The eddy covariance technique is used as a possible solution to estimate CO2 emissions from the Vuwani area. The method measured the exchange of CO2 between the surface and the atmosphere and provided accurate and continuous measurements of daily means of Net Ecosystem Exchange ranging from -5 gCmˆ(-2)/day and +54 gCmˆ(-2)/day that included meteorological parameters radiation (daily mean) of minimum 250 w.m-2 and maximum 504 w.m-2. The daily CO2 flux ranged from ± 7 µmol/mˆ2 sˆ1, and close to 100% energy closure. The findings of this study assist in formulating policies and strategies to reduce CO2 emissions in rural areas and mitigate climate change.

Keywords: Vuwani area, climate change, Net ecosystem exchange, CO2 emissions, eddy covariance

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics of Condensed Matter and Materials Track 1 / 173

Density Functional Theory Study of Zn Doped CsPbI3 Perovskite for Photovoltaic and Optoelectronic Applications

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Co-authors: David Tshwane [2]; Martin Ntwaeaborwa [3]; Maphanga Regina [2]

[1] *Yes*

[2] *CSIR*

[3] *University of Witwatersrand*

Corresponding Author: prettier.maleka@gmail.com

The structural, electronic, and optical properties of the undoped and transition metal Zn doped CsPbI3 were investigated using first-principles calculations within the framework of spin polarised density functional theory implemented in VASP code. The calculations are performed using the local spin density approximation GGA+U method in order to correct the strong Coulomb interactions of 3d electrons. The substitution of Pb atom with the Zn atom reduces the bond length and lattice constants of CsPbI3 due to Zn atom having a smaller ionic radius compared to the Pb atom. The calculated band gap of undoped CsPbI3 is a direct band of 1.488 eV and of Zn doped is an indirect band gap of 0.717 eV. radiation indicate that the materials could be good candidates for solar cell applications. The study of the mechanical properties demonstrates that Zn doped material is mechanically stable and ductile nature as the undoped CsPbI3 compound.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 1 / **174**

Proton beam and femtosecond laser writing lithography method for semiconductor microstructures

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Co-authors: Chester Kotsedi [2]; Mark Blumenthal [1]; Nametso Mongwaketsi [2]

[1] *University of Cape Town*

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We herein report on the fabrication of patterns using proton beam writing (PBW) and femtosecond laser lithography. In femtosecond laser lithography, high-resolution patterns can be created on semiconductor materials using the energetic photons from a laser source as it has been done for the fabrication of microfluidic lab on chip photonic devices and biochips applications. In the pattern fabrication for this study, a femtosecond laser with a wavelength of 1034 nm, a repetition rate of 200 kHz, and a pulse duration of 190 fs will be used. The structures will be created using pre-programmed in the X-Y stage controller software.On the other hand, PBW uses focused high-energy beams of protons to probe the material to fabricate patterns or structures at the micro- and nanoscale. This will be achieved using a 3MV Tandetron accelerator at iThemba LABS, proton beam focusing is achieved by using Oxford triplet quadrupole lenses and scanning uses an electrostatic scanning system positioned in front of the lenses. In contrast to femtosecond laser writing, PBW tends to have a deeper penetration into the target material due to the higher energy of the protons, which leads to three-dimensional structures with higher sub-micrometer precision. Patterns were created on a PMMA using 3 MeV protons and the fluence was counted as electrical charge per unit monitored by exposure time, beam current, and irradiated area. A Femtosecond laser was also used to fabricate the cross-like patterns from pre-programmed patterns by focusing a laser pulse onto PMMA for comparison. The morphological and microstructural characterization of the samples was

conducted using scanning electron microscopy (SEM) and atomic force microscopy (AFM). The fabricated cross-like patterns will be used in a study of low-temperature Hall bar measurements for device fabrication.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Consent on use of personal information: Abstract Submission:

Poster Session 2 / **175**

Ion-induced radiation damage in Lutetium-Aluminium and Gold using SRIM-2013

Author: Samuel Terungwa Temaugee[1]

Co-authors: Iyabo Usman [2]; Risimati Dazmen Mavunda [3]

[1] *School of Physics, University of the Witwatersrand, Johannesburg*

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[3] *UJ / Wits*

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The Monte Carlo simulation Code, Stopping Power, and Range of Ions in Matter (SRIM) has been effective among other binary collision approximation codes for estimating the level of damage produced due to ion irradiation in materials. This study estimated the level of damage by heavy and light-ion irradiation to Lutetium-Aluminium (Lu-Al) and gold materials with Au and proton ion implantation respectively using SRIM-2013 quick damage simulations. Lu-Al and Au have applications in reactor flux monitoring, advanced space, and collider systems. There has been growing evidence that protons and much more heavy-ion irradiation produces displacement damage effects comparable to that of neutrons on the microstructure of irradiated materials. Hence, this present study of the effect of light and heavy ion irradiation will contribute to the current understanding of ion irradiation in the materials of choice. Total damage in the materials was computed at the Primary Knock-on Atom (PKA) energies of 0.02, 0.1, 0.4, 0.5, 1.0, and 10.0 MeV. Damage profile results revealed that irradiation with Au-ions produced more damage to the materials than proton-ions at the same PKA energies. Also, the damage levels increased with increasing PKA energies. Frenkel pairs produced due to ion implantation in the Au material were also seen to be higher than in the Lu-Al Alloy.

Keywords: Ion-irradiation, microstructure, SRIM, proton, radiation damage.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Photonics / **176**

Real-time feedback-driven single-particle tracking spectroscopy of LHCII

Authors: Bertus van Heerden[1]; Tjaart Krüger[1]

[1] *University of Pretoria*

Corresponding Author: bertus.vanheerden@up.ac.za

Single-molecule spectroscopy (SMS) has proven to be a powerful technique for investigating structure-function relationships in light-harvesting systems. In particular, SMS has unraveled dynamics in light-harvesting complexes that are hidden in ensemble measurements. However, the environment used in SMS experiments is a poor representation of the natural cellular environment, and therefore the results of these studies may be of limited physiological relevance. One limitation of conventional SMS experiments is the need to immobilize the complexes via surface attachment or to trap the complexes using, e.g., an anti-Brownian electrokinetic (ABEL) trap. This limitation is overcome by real-time feedback-driven single-particle tracking (RT-FD-SPT), a non-invasive technique that allows SMS measurements to be performed on single, freely diffusing particles for extended durations and with excellent spatiotemporal resolution. We studied different RT-FD-SPT methods using statistical analysis and simulations before using RT-FD-SPT to experimentally measure fluorescence lifetimes and emission spectra of single diffusing plant LHCII complexes. This paves the way for studies of the effect of surface immobilization as well as for studying single LHCII complexes in close-to-natural environments.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Photonics / **177**

Curcumin an emerging natural photosensitiser for lung cancer photodynamic therapy

Author: Glory Kah[1]

Co-authors: Heide Abrahamse [1]; Rahul Chandran [1]

[1] *University of Johannesburg*

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Abstract. Worldwide, lung cancer remains the main cause of malignant tumours and it contributes to a high mortality rate in cancer cases. Conventional therapeutic approaches for lung cancer are characterised as ineffective since resistance to therapy and toxic after-effects do occur in patients. Photodynamic therapy (PDT) is a promising therapeutic approach that requires a specific light source for the activation of a photosensitiser to induce cytotoxic cell death via the generation of reactive oxygen species. Curcumin is a natural compound from Curcuma longa that has been confirmed as a photosensitiser. This study aims to investigate the in vitro effects of curcumin-mediated PDT of lung cancer. Lung cancer cell lines (A549) were grown in complete media in an incubator maintained at

85% humidity, 5% CO2, and a temperature of 37℃. Treatment of cells was achieved by exploring different concentrations of curcumin, and the cells were irradiated with a 470 nm diode laser at 5 J/cm2 fluency. Post-PDT tests including microscopic evaluation of treated cells and biochemical analysis were performed to determine the cellular response of cells treated. The results revealed morphological alterations and decreased viability in treated cells, which signifies cytotoxic damage. Thus, the increased cytotoxic effect established in this study suggests that curcumin can be an effective natural photosensitiser over synthetic ones for mediating lung cancer PDT. Further in vivo studies may be needed to evaluate how curcumin can be utilized for lung cancer PDT in clinical settings.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Theoretical and Computational Physics / 178

Wave Mechanics for Dissipative Classical Systems

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Co-author: Sekhants'o Lara [1]

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Dissipative systems are among the most interesting and challenging systems to study in physics. For instance, they require non-standard (i.e. complex) Lagrangians which include velocity-dependent potentials coupling the system of interest to another system (i.e. the environment). That is, a dissipative system can be thought of as a system that is coupled to another system. As such, studying this kind of system can only be complete if both (coupled) system units are studied together. This paper considered such a dissipative system and demonstrated a derivation of a wave equation governing its dynamics. Comparing the resulting wave equation to Schroedinger's wave equation proved Schrodinger's wave equation as a special case of the derived wave equation. A classical RLC circuit was modeled and analyzed within the framework of the derived wave equation and the resulting measurement loading was compared (at least conceptually) to the quantum measurement back-action. The paper then drew some inferences and speculated on the possibility of a quantum particle being interpreted as a dissipative particle coupled to its image (i.e. identical partner) particle in the dual space; that is, more like a self-interacting particle.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 2 / 179

Density functional theory study of transitional metal doped ZnO nanostructures for gas sensing: Interaction of NH3 and NO2 with the doped ZnO surface

Authors: Matimu Makhubele[1]; Ratshilumela Steve Dima[2]; Rapela Maphanga[3]; Nnditshedzeni Eric Maluta[1]; Joseph Kirui[4]

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The adsorption and interaction mechanisms of gaseous molecules on ZnO surfaces have received a substantial amount of attention recently as a direct result of the technical uses that they offer in gas sensing. The adsorption behaviour of molecules of NH3 and NO2 was examined using density functional theory on surfaces of undoped and M-doped ZnO (101) where (M = Ni, Co, and Cu). It was discovered that each of the adsorption energy values had a negative value, which suggests that both molecules absorb through the process of chemisorption rather than physisorption. According to the results of the adsorption energy calculations, the molecule of NH3 has an energetic profile that is more compatible with adsorption on the exposed ZnO surface than the NO2 molecule does. On the other hand, it was found that the surface of all the M-doped ZnO could support a robust adsorption arrangement for the NO2 molecule. The redistribution of charge density showed that the adsorbent and the adsorbate each had charge accumulation and depletion on their respective surfaces. The density of states and band structures were also studied in order to study the electronic behavior of molecules of NH3 and NO2 that had been adsorbed on surfaces of undoped and Sn-doped ZnO (101), respectively.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

MSC

Physics for Development, Education and Outreach / **180**

Biogas upgrading and bottling

Authors: Patrick Mukumba[None]; Yolanda Mapantsela[None]

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ABSTRACT
The production of biogas in South Africa is gaining popularity as a sustainable solution to waste management and energy production. However, the biogas produced from organic waste needs to be upgraded biomethane to meet the required specifications for use as fuel for road transport, electricity generation, and or for injection into the national gas grid. Biogas is a renewable energy fuel that is produced from the anaerobic digestion of organic matter, such as agricultural waste, food waste, sewage sludge, and other organic materials. It is a mixture of gases, mainly methane and carbon dioxide with small amounts of other gases such as hydrogen, nitrogen, and hydrogen sulfide. Biogas can be purified to meet natural gas quality standards. The commercial upgrading and purification technologies of biogas exist in the world for large-scale biogas plants. However, there are no such commercial purification technologies available for small-scale biogas digesters, mainly found in rural communities.
This research aims to provide an overview of the potential of biogas upgrading, purification, and bottling in South Africa. It highlights the challenges faced by the country on biogas upgrading and discusses potential solutions to accelerate the development of biogas upgrading, purification, and bottling system. A portable biogas digester with a portable upgrading, purification, and bottling system is also designed in this research.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

Msc

Nuclear, Particle and Radiation Physics / **181**

Ra-226 on the deterioration crosswalk speed bumps of rural and township ships road in Vhembe region, Limpopo Province.

Author: Nemangwele Fhulufhelo[1]

Co-author: Tshenzhemo Mudau [2]

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Deterioration of pavement condition near and on the speed, bumps is observed throughout South Africa, mainly in rural and townships area. The material used to construct those speed bumps is found to be radioactive with a considerable dose rate of 0.9μSv/h compared to the 1000μSv annual limit for radiation exposure for a public member. The hazard posed by skin exposure from Ra-226 is, therefore, due primarily to its daughter products which include several high-energy alpha, beta, and gamma emissions. Beta radiation significantly contributes to skin dose at the nominal skin depth of 70 μm from Ra-226 and its progeny.

Keywords: Ra-226, Skin exposure, Beta radiation, Dose rate, Construction material

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Nuclear, Particle and Radiation Physics / **182**

Recent Progress in the South African contribution to the ATLAS Tile Calorimeter Phase-II Upgrade at CERN

Author: Edward Nkadimeng[1]

Co-authors: Ryan Mckenzie [2]; Tristan Jade Wilkinson [1]; Khathutshelo Phadagi [3]; Mpho Gift Doctor Gololo [4]; Bruce Mellado [5]

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The Large Hadron Collider (LHC) at CERN is a cornerstone of modern particle physics research, and the ATLAS experiment is one of the largest and most complex detectors at the LHC. The upcoming Phase-II Upgrade of the ATLAS detector presents a major opportunity for advancing our understanding of the fundamental properties of matter and the universe. South African institutions are playing a key role in the Phase-II Upgrade of the ATLAS Tile Calorimeter, with contributions to both on-detector and off-detector electronics. South African institutions are contributing significantly to the Phase-II Upgrade of the Tile Calorimeter at the LHC, with 50% of the production of the Low Voltage Power Supply Bricks (LVPS) and 24% of the production of the Tile Preprocessor (PPr) being fully manufactured and tested in South Africa. This talk will provide an overview of the South African contribution to the Phase-II Upgrade of the ATLAS Tile Calorimeter, including the design, manufacturing, and testing of the LVPS bricks and PPr boards, as well as the benefits to South African students and researchers involved in the project.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Nuclear, Particle and Radiation Physics / **183**

High Energy Neutrons at the NRF-iThemba LABS

Author: Peane Maleka[1]

Co-author: Zina Ndabeni [2]

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iThemba Laboratory for Accelerator Based Sciences (iThemba LABS) is a national facility of the National Research Foundation (NRF) in the Republic of South Africa. Activities at iThemba LABS are based around a number of sub-atomic particle accelerators located at the Cape Town and Johannesburg campuses. The largest of these, a K=200 separated sector cyclotron (SSC), accelerates protons to energies of 200 MeV, and heavier particles to much higher energies. These instruments and setups provide opportunities for modern research, advanced education and the production of unique radioisotopes [1]. The iThemba LABS neutron beam experimental facility is one of the few facilities available worldwide to provide quasi-monoenergetic neutron beams in the energy range, 30 MeV to 200 MeV [2]. Quasi-monoenergetic neutron beams in this range are produced in the neutron experimental vault via the 7Li(p,xn) or 10Be(p,xn) reactions [3] for varying thicknesses of Li and Be targets. Collimated fan beams are possible at neutron emission angles amongst others of 0° and 16°. These neutron beams at iThemba LABS have been well characterized [4,5]. The facility is currently designated by the National Metrology Institute of South Africa as an entity responsible for providing traceability for the medium and high-energy neutron measurements in South Africa. Thus, the facility is intended to support neutron physics research and metrology communities for calibrations of neutron detectors and radiation protection instruments. Cross-section measurements for neutron-induced reactions in the medium to high-energy region can also be performed.

For this contribution, we present some of the ongoing developments and future plans of the facility.

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Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Applied Physics / **184**

A physics approach to ecological networks

Author: Alan Matthews[1]

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An ecological network is typically a system of nutrient transfer between groups of species in an ecosystem. In common with physics, energy and mass are conserved, and transfer across the ecosystem boundaries are tracked. Furthermore, ecologists are concerned with macroscopic variables that characterise the system, including an analogy of entropy to measure the degree of order. Mathematically, a static network is a combination of constraints and degrees of freedom. A prominent method of solution is a linear inverse model that finds a solution space that includes unphysical negative flows which must be excluded. An alternative approach is to ensure from the outset that all flows are positive. Ecological networks are important in themselves, and also serve as models for efficient networks in other domains such as energy distribution.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Applied Physics / **185**

Introducing the 10kW Solar Trough Prototype

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This paper introduces our newly constructed solar trough collector featuring a cavity-type receiver design. This prototype has a receiver area of approximately 10kW, and includes an innovative focal length arrangement tailored for cavity-type receivers. A high-temperature pump is used to circulate a mineral oil as the heat transfer fluid. The receiver design incorporates a highly reflective inner

cavity wall, encased by a vacuum sleeve, which helps to minimize thermal radiation losses. The unit can be controlled using a web application, with remote temperature sensors providing data collection capabilities in the cloud, and the mechanics controlled by an IoT web. Initial temperature measurements have been taken, and the efficiency values will be presented.

Apply to be considered for a student ; award (Yes / No)?:

no

Level for award;(Hons, MSc, PhD, N/A)?:

na

Poster Session 1 / **186**

Self-Consistent Charge Density-Functional Tight-Binding Parameterization for the Mg–Si system

Authors: Simon Maphanga[None]; Katlego Phoshoko[1]; Phuti Ngoepe[1]

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Lithium-ion batteries have been widely used as a solution for portable energy storage over the years, however, the rising demand for high-energy-density batteries calls for the design of new high-performing electrode materials. Magnesium-based batteries emerged among alternatives to lithium-ion batteries, however, further studies are still required to help accelerate developments toward their commercialisation. In this work, we present the self-consistent charge density-functional tight-binding (SCC-DFTB) parameterization of the Mg-Si system. The developed parameters are validated against available experimental data and calculated DFT results using Mg, Si and Mg-Si systems. The structural properties obtained by applying the parameter set show good agreement with the experimental values, and by modelling the electronic properties of the Mg₂Si supercell the set is shown to handle large systems. The Mg-Si SCC-DFTB parameters from this work paves the way for further investigations, as they will make it possible to study and predict the behaviour of Mg-Si-based electrode materials through computer simulations.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Photonics / **187**

Modelling linear spectra of plant light-harvesting complexes

Author: Johan Nöthling[1]

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During the initial stage of photosynthesis, sunlight is absorbed by molecular light-harvesting complexes. The technique of linear optical spectroscopy is a powerful tool to study these complexes. In principle, all the information contained in an experimental linear spectrum can be extracted through comparison with the corresponding modelled spectrum—provided that the modelling is accurate. In this presentation, we discuss the physics underlying linear spectroscopy and how these spectra can be modelled. We consider an exact method based on stochastic path integration (PI) and several approximate methods, including the Full Cumulant Expansion (FCE), complex time-dependent Redfield (ctR), Redfield, and modified Redfield methods. We characterize the accuracy of the approximate methods for modelling absorption- and fluorescence-type linear spectra by comparing the approximate spectra with exact spectra for a model system similar to plant light-harvesting complexes. We show that the FCE method performs best for absorption-type spectra but, surprisingly, may break down when calculating fluorescence-type spectra. We also show that the often-used Redfield and modified Redfield methods both perform poorly. We consider two applications of linear spectral modelling. First, we use particle swarm optimisation (PSO) to fit the experimental spectra of the plant light-harvesting complex CP29 with modelled spectra. Based on the molecular parameters producing the best fit, we show that CP29 likely has a dual role as an excitation conduit and as a dissipater of excess energy. As a second application of spectral modelling, we train neural networks to predict disordered linear spectra from molecular parameters and *vice versa*. We show that the neural network models can make accurate predictions orders of magnitude faster than the traditional modelling methods.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics of Condensed Matter and Materials Track 2 / 188

Variation of Statistical Ensembles to Optimise Complex Core-Shell Cathode Models: A Molecular Dynamic Approach

Authors: Precious Makhubela[None]; Raesibe Ledwaba[None]

Co-authors: Phuti Ngoepe ; Kenneth Kgatwane

Corresponding Author: pgmakhubela@gmail.com

The O3-type Li2MnO3 is one of the potential replacements of the expensive nickel and toxic cobalt-based cathode materials for the portable, high power and high energy density lithium-ion batteries. However, Li2MnO3 suffers structural instability during cycling. Surface coating of cathode materials has sparked attention and has modified most of the commonly used cathode materials. The O3-type Li2MnO3 layered has been investigated over the years as a coating material for other cathodes but never as the core material. The O2-type Li0.69MnO2 is of great interest because unlike other lithium manganese oxides, it does not transform into a spinel structure during cycling and its conductive property enables it to allow undisturbed movement of Li atoms during battery operation. This study explores firstly the tedious process of modelling and developing core-shell systems that are meant to serve as electrode material with coating interface. The second aspect of interest is optimising the simulation conditions for molecular dynamic simulations of these core-shell systems. A core-shell model of the Li2MnO3-Li0.69MnO2 system is presented and preliminary molecular dynamics results are demonstrated under different ensembles. The Li2MnO3-Li0.69MnO2 core-shell structure was slightly disordered under the ensembles NPT, NST, and NVT. The radial distribution function plots indicated the bonding length to be 2Å between the manganese and oxygen from both the core and shell through the different ensembles.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Nuclear, Particle and Radiation Physics / **189**

Update on the multi-lepton anomalies and scalar candidates at the LHC

Authors: Bruce Mellado[1]; Salah-eddine Dahbi[2]

Co-authors: Srimoy Bhattacharya [3]; Mukesh Kumar [1]

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[2] *University of Wits*

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In this presentation we give an update of the multi-lepton (electrons and muons) anomalies at the LHC is given. These include the excess production of opposite sign leptons with and without b-quarks, including a corner of the phase-space with a full hadronic jet veto; same sign leptons with and without b-quarks; three leptons with and without b-quarks, including also the presence of a Z. The internal consistency of these anomalies and their interpretation in the framework of a simplified model are presented, where the inconsistency of the data with the SM is more than 8σ. The simplified model includes a singlet scalar S with a mass in the range 130-170 GeV produced from the decay of a heavier new scalar H, leading to di-boson signatures. Motivated by this, a search for narrow resonances with S$\rightarrow\gamma\gamma$, Zγ in association with light jets, b-jets or missing transverse energy is performed. A narrow excess is found at 151.5 GeV with a global significance exceeding 5 sigma, including recent results from the LHC experiments. The connection with the 96 GeV candidate is also discussed.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Theoretical and Computational Physics / **190**

Studying the dependence of observables on the impact parameter (b) in Pb+Pb High Energy Heavy-Ion collision particle multiplicity from the microscopic model (UrQMD) at Elab = 300 AGeV.

Authors: Thendo Emmanuel Nemakhavhani[1]; Azwinndini Muronga[1]; Alex Mothibi[2]; Connie Machema[3]; Tshimangadzo Mbabala[4]

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[4] *Wits University*

Corresponding Author: tnemakhavhani@uj.ac.za

The impact parameter dependence (b = 0 − 19%) of different meson and baryon species at central rapidity and particle ratios in Pb+Pb was studied employing High Energy Heavy-Ion collisions at an incident kinetic beam energy (lab frame) of Eelb = 300 AGeV for a duration of t = 400 fm/c. The Pb+Pb reaction was simulated from the Ultra-relativistic Quantum Molecular Dynamics model (UrQMD). We employed the particle ratios technique to distinguish between hadronic cascade and hydrodynamical models, incorporating a QGP phase transition. The study will give an insight into the behaviors of particle production at different impact parameters leading to chemical freezeout and thermal equilibrium. This will open more windows when it comes to a better understanding of the phase transition of the hadron gas for different High Energy Heavy-ion collision systems. We report here on the results at central rapidity and above the saturation time, at a randomly chosen time of t = 380 fm/c, and also the particle ratio as a function of impact parameter at a different time t for both meson and baryon species.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / 191

Configuration of power chips for the TileCoM for Phase-II Upgrades at CERN.

Author: Mpho Gift Doctor Gololo[1]

Co-authors: Claudia Tsema ; Bruce Mellado [2]

[1] *Witwatersrand University*

[2] *University of the Witwatersrand and iThemba LABS, National Research Foundation*

Corresponding Author: mgd.gololo@gmail.com

The Large Hadron Collider (LHC) has four main experiments along the ring. The ATLAS (A Toroidal LHC Apparatus) experiment along with the other three experiments enables the physicists to analyze collected data. The Large Hadron Collider needs to be upgraded to a High Luminosity Large Hadron Collider (HL-LHC) to account for the increase in luminosity and to enable physicists to explore phenomena beyond the standard model. South Africa contributes to the upgrade of the LHC. The contribution involves the production of the GbE switch and TileCOM Printed Circuit Board (PCB) which connects the Phase-II upgrade electronic chain to the network to monitor and allow for data transmission at high speeds. As part of the production, components such as TPS65086100 are required to be configured before the population on the TileCoM PCB. This research paper illustrates the methodology followed to configure power chips (TPS65086100) and the plot results in terms of regulated voltage and currents.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Applied Physics / 192

Applications of Graph Neural Networks in Particle Physics and Air Quality Systems for PM2.5 forecasting

Author: Craig Rudolph[1]

Co-authors: Bruce Mellado [1]; PAllab BAsu [2]

[1] *University of the Witwatersrand*

[2] *Senior Lecturer*

Corresponding Author: craig.rudolph@cern.ch

Graph Neural Networks (GNNs) are widely used in particle physics research as a solution to handling complex, sparse, and noisy data. Detectors capture millions of measurements per second, resulting in high-dimensional data that is difficult to analyze.
GNNs allow us to model data as a graph, where each detector component corresponds to a node and edges represent interactions between particles. Message-passing algorithms propagate information throughout the graph, allowing GNNs to capture complex relationships between detector components and learn representations of physical processes.
GNNs are used for particle identification, event reconstruction, and anomaly detection, and can also be used for air quality systems to predict pollutant concentration.
In air quality systems, the graph consists of air monitoring stations measuring pollutant concentration and meteorological data every hour. Each monitoring station corresponds to a node and edges represent how stations interact. The graph is constructed based on how stations transport PM2.5 concentrations to each other. The adjacency matrix defines which nodes are adjacent to each other based on factors that hinder the transport of PM2.5, such as distance, mountain ranges, and elevation differences. Edges contain information about wind speed, wind direction, distance, and the direction of the source station to the sink station.
This improves the accuracy of the prediction.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / 193

Kernel density estimation and weakly supervised machine learning-based models for Higgs-like signals data classification

Author: Nidhi Tripathi[1]

Co-author: Bruce Mellado [2]

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[2] *University of the Witwatersrand*

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Following the anomaly observed in multi-lepton final states through the decays of heavy scalar resonance in ⌧⌧ data at the Large Hadron Collider via proton-proton collisions, we develop a Kernel density estimation-based machine learning model to generate synthetic dataset. The dataset comprises SM Higgs-like signals such as ggF, VBF, WH and ZH. Further we use weak supervised machine learning methods and deep neural network model(s) to classify and discriminate between original

and synthetic dataset. We demonstrate the ability of this approach to reproduce the various kinematic observables in the said final states, and preliminary results shows that this model generates the synthetic data reasonably well, where the performance is compared with the standard samples using Monte-Carlo event generators.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / **194**

Gas sensing mechanism of Ethylene on pure Co3O4 (311) surface: Density Functional Theory Study

Author: Modjadji Rebecca Letsoalo[1]

Co-authors: Steve Ratshilumela Dima [2]; Nnditshedzeni Eric Maluta [3]; Katekani Shingange [4]

[1] *University of Venda*

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Advanced sensing technology is required for the detection of gases and volatile organic compounds (VOCs) for application in environmental monitoring, disease diagnosis, and smart agriculture. Among the many materials used as sensing layers, nanostructured semiconductor metal oxide-based sensing materials have recently gained preference owing to their outstanding sensitivity and high surface area. The flexibility to tune their morphology and surface characteristics also add upon to their most use in this field of gas sensors. Considerable experimental research has shown the behaviour of the semiconductor metal oxide-based gas sensors towards different gases; however, they do not provide a detailed understanding of the sensing mechanism. This work focuses on density functional theory (DFT) calculations to explore the electronic properties of the bulk Co3O4 and its (311) surface using the BIOVA Material Studio. The general sensing mechanism describing the performance of Co3O4 when exposed to ethylene molecules is also discussed.

Key words: Gas sensor, nanostructured, Co3O4, DFT calculations, ethylene, sensing mechanism

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Applied Physics / **195**

O2 adsorption on PtSb2 (100) surface

Authors: Samuel Mangwejane[None]; Peace Mkhonto[1]; Phuti Ngoepe[1]

[1] *SAIP*

Corresponding Author: seshupo.mangwejane@ul.ac.za

In order to understand the oxidation of the PtSb2 minerals by either weathering or exposure to air, we considered the adsorption of oxygen molecules on mineral surfaces. The adsorption properties will give more insight into the interaction of the oxygen with the atoms on the surface. Generally, minerals are exposed to atmospheric air during crushing or storage. It had been reported previously that oxidation depresses sulphide minerals, resulting in poor grade-recovery performance and the brittle nature of PtSb2 may result in difficulty of its recovery from such ores. The surface energy of (100) has been found to be 0.920 Jm-2 as compared to (110) 1.194 Jm-2 and (111) 0.939 Jm-2. We performed oxidation on the PtSb2 (100) surface where O2 was adsorbed in a peroxo, superoxide and Pt-O-O-Sb bridging on the surface Pt and Sb atoms.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Consent on use of personal information: Abstract Submission:

Poster Session 2 / 196

Setting up an environment for extracting and analyzing data from the DCS ATLAS experiment for the behavior of High Voltage channels

Author: Sanele Scelo Gumede[None]

Co-authors: Betty Kibirige ; Filipe Martins ; Juraj Smiesko [1]; Lungisani Phakathi

[1] *Charles University, Faculty of Mathematics and Physics, Institute of Particle and Nuclear Physics*

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A hadronic calorimeter called Tile Calorimeter (TileCal) can be discovered in the center of the ATLAS detector. A sample calorimeter called TileCal employs steel plates as the absorber and plastic scintillating tiles as the active medium. Because about 30% of the total energy jets produced in a proton-proton collision are deposited in TileCal, it is crucial in the accurate reconstruction of the kinematics of the physics events. The main objective of this project is to develop the plugin that will be used to retrieve data from the Detector Control System (DCS) Data Viewer server and analyze it for anomalies in the HV channels. The plugin will then be incorporated into the Tile-in-One platform, which unifies all TileCal work onto a single platform

Apply to be considered for a student ; award (Yes / No)?:

no

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Consent on use of personal information: Abstract Submission:

Astrophysics & Space Science / 197

Commensal searching for radio transients/variables in MHONGOOSE Large Survey Project (LSP).

Author: Vhuthu Tshilengo[1]

Co-authors: Patrick Woudt [2]; Eric Maluta [1]

[1] *Univen*

[2] *UCT*

Corresponding Author: tshilengov@gmail.com

Commensal searching for radio transients/variables in MHONGOOSE Large Survey Project (LSP).

The MeerKAT radio telescope is the newly built South African precursor radio telescope array for the mid frequency component of the Square Kilometre Array (SKA1-Mid). Its excellent sensitivity and wide field of view, combined with commensal access to a large number of MeerKAT surveys, allows astronomers to gain new insights in time-domain radio astronomy, particularly in uncovering the population of faint radio transients and variables. In this study use the SARAO SDP (Science Data Processing) images of observations of the MHONGOOSE Large Survey Project (LSP) to search for new radio transients. MHONGOOSE is targeting 30 different galaxies (pointings) observed over 10 epochs per pointing. The aim of this project is to search a selection of MHONGOOSE fields for radio transients / variables over the 10 epochs per field. We used the Transient Pipeline (TraP) on the cloud compute infrastructure of the Inter-University Institute for Data Intensive Astronomy (IDIA) to characterise the light curves of point sources in the field using statistical variability parameters. Here we show the first results of our search for radio transients in the MHONGOOSE data set of NGC 1566.

Keywords: Transients; Variables; Radio Astronomy

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Consent on use of personal information: Abstract Submission:

Poster Session 1 / 198

Understanding the origin of Bunny-Hop light curves of periodic methanol masers

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Corresponding Author: andreanel101@gmail.com

Class II 6.7 GHz methanol maser emission, first discovered by Menten (1991), is exclusively associated with high-mass star-forming regions. Long-term observational studies have shown that masers are variable on many timescales; this finding was unsurprising as masers are incredibly sensitive to the changes in their local physical environment. A more surprising finding was that of the periodic methanol masers originally reported by Goedhart et al. (2003) and Goedhart et al. (2004). There are now close to thirty periodic maser sources known to us. In this research, the methanol maser source

G358.460 - 0.391 was observed using the 26-metre HartRAO telescope to characterise its periodic nature; the maser is periodic, and the periodic nature of the light curve follows a behaviour which can best be described as an absolute cosine behaviour; such sources have been termed \textit{bunny-hop} sources. The source was also observed to have a velocity drift, and based on observations completed in this project as well as recent literature, it is believed that the maser region has a face-on orientation, i.e, the accretion disc associated with the high-mass stellar object is orientated face on with bipolar outflows in the direction of the observer. It is believed that the distinct periodic nature of the maser is due to some well-behaved periodic behaviour within the maser environment, and the face-on orientation may be correlated to the district bunny-hop behaviour observed.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Consent on use of personal information: Abstract Submission:

Poster Session 2 / 199

Numerical study of a metallic fluid flow in a magnetohydrodynamic pump

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Co-authors: Gideon Wiid [2]; Shane Martin [3]; Kessie Govender [3]

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A magnetohydrodynamic (MHD) pump is a device that can move/pump a metallic fluid by utilizing an electric current together with a magnetic field. The operation of the pump is based on the principles of an electrically conductive fluid that is exposed to electromagnetic forces. When a metallic fluid passes through the device, the current and magnetic field combine to produce the Lorentz force. This force is responsible for the pump's operation and can be harnessed for various industrial and energy applications. The advantage of the MHD pump over traditional mechanical pumps is that, besides the working fluid, it operates with no moving parts.
Mercury has been used as a working fluid in magnetohydrodynamic pumps since the early years of its development in the 1960s. Galinstan, an alternative liquid metal with similar properties, is now widely used in MHD pumps. The switch to Galinstan from mercury was made due to concerns over the toxicity and environmental impact of mercury. This change was a result of extensive research to find a safer and more environmentally friendly substitute for mercury in MHD pumps. As a result, there are numerous new applications of the MHD pump and this research endeavours to study the flow properties of the fluid in small-scale applications.
In the present study, we investigate the properties of the fluid flow in the MHD pump using numerical techniques. This is a precursor to developing a measurement technique thereafter to experimentally study the flow properties. As a first step, we numerically solve the fluid equations to gain insight into the behaviour of the working fluid under various operating conditions. The initial investigation will discuss the motion of a single particle in the presence of an electric and magnetic field. This will be followed by the numerical simulation of the MHD fluid equations. The numerical simulation will be a set of differential fluid equations that are discretized using the finite difference method and solved in MATLAB by using standard programming practices. The results will be presented for the various scenario-based simulations.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 2 / 200

Comparative performance analysis for optimally designed on-grid and off-grid hybrid power systems for a Limpopo, South Africa Community Development Centre energy system

Author: Shandukani Muronga[None]

Co-authors: DAVID TINARWO [1]; Sophie Mulaudzi [2]

[1] *UNIVERSITY OF VENDA*

[2] *University of Venda*

Corresponding Author: murongashandukani8@gmail.com

The current global energy crisis is threatening sustainable development. In South Africa, the continuous increase in power outages (load shedding) is crippling the country's economic growth, as evidenced by the recently witnessed closure of several small businesses. An avalanche in implementing different renewable energy technologies has been witnessed, with several residential buildings and firms turning their roof space to photovoltaics renewable energy generators. Local municipalities have different by-laws for connecting distributed renewable energy generators to the local grid, making it difficult to implement these PV systems . Additionally, PV systems configurations require an understanding of optimal configuration and proper scheduling to match the load demand. Thus, off-grid grid-tied, and grid-interactive hybrid PV energy systems design, scheduling and performance analysis are gaining increasing attention from academia and industry to enhance their integration as an alternative energy source. However, choosing the most appropriate system configuration for specific load characteristics, especially when the utility grid is available, can result in losses due to sub-optimal planning and operational strategy. This study aims to provide a comprehensive understanding and fill the knowledge gap on grid-connected photovoltaic and hybrid power systems design and operation using Masia Development Center, Limpopo as a case study . The idea of this study is not to claim or confirm the performance of an installed PV system but to show the feasibility of off-grid and grid-interactive hybrid renewable energy system (HRES) in a residential house or on a small scale. The solar resource data for this study were analysed for PV applications. Load characteristic data of the system were collected and used for optimisation simulations with a hybrid electric renewable energy optimisation model (HOMER). Different dispatch strategies were applied to determine the optimal configuration for the three most common PV system configurations (off-grid/isolated hybrid and grid-tied) per case. The study aims to help residents, non-profit organisations, and the government better share scarce resources to achieve energy goals and meet Sustainable Development Goal (SDG) , ensuring access to sustainable, affordable, reliable, and modern energy.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Consent on use of personal information: Abstract Submission:

Nuclear, Particle and Radiation Physics / 201

Operations of the ATLAS Hadronic Tile-Calorimeter

Author: Ryan Mckenzie[1]

Co-author: Bruce Mellado [2]

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The Tile Calorimeter (TileCal) is a sampling hadronic calorimeter covering the central region of the ATLAS detector. The TileCal provides important information for reconstruction of hadrons, jets, hadronic decays of tau leptons, missing transverse energy and assists in muon identification. The annual operation of the TileCal follows that of the ATLAS detector and by extension the Large Hadron Collider (LHC). The LHC schedule is segmented into discrete periods defined and agreed upon by the LHC and the experiments located along its circumference. This talk will present the activities of the TileCal collaboration that took place from last period of physics data taking in 2022 up until the first stable beams in 2023. A chronological approach will be used to provide insight into the operation of the TileCal with key milestones such as the Year-End Technical Stop, detector calibration, detector commissioning, dedicated tests, beam splash events and the first stable beam collisions being covered.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics for Development, Education and Outreach / **202**

Low-cost methods and devices to measure the heat capacity of gases.

Author: Marco Mariola[1]

Co-author: B Martincigh [2]

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[2] *Universtiy of KwaZulu-Natal*

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The measure of the heat capacity of gases is one of the fundamental experiments in scientific disciplines. Usually, the determination of the heat capacity requires the knowledge of the speed of sound. To measure the speed of sound, the classical experimental setup consists of a Knundt's tube, one oscilloscope, and a function generator to determine the wavelength of the wave. While the Knundt's tube can be relatively easy to replace with Do It Yourself materials, the function generator and the oscilloscope are still the most expensive part of the experimental setup. This experiment, oriented for educational purposes, doesn't require high-level precision instruments, and possible alternatives to an oscilloscope and function generators are possible. In the presented work, two low-budget instrument alternatives are presented.
The possibility to reduce the budget is an opportunity to introduce new laboratory activities in secondary schools or a case of necessity in the tertiary institutions.

Apply to be considered for a student ; award (Yes / No)?:

N

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Applied Physics / 203

An Internet-Of Things pilot project as a primer for future technological development for high-energy physics detector control systems.

Author: Ryan Mckenzie[1]

Co-authors: Bruce Mellado [2]; Carlos Solans Sanchez [3]; Tristan Jade Wilkinson [4]; Ling Cheng [5]; Cameron Baldwin [5]

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[2] *University of the Witwatersrand and iThemba LABS, National Research Foundation*

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[4] *University of the Witwatersrand*

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Detector Control Systems (DCS) and Data AQuisition (DAQ) Systems are susceptible to technological development due to the intricate relationship between their design and currently available hardware. This when coupled to the manner in which particle detectors are required to evolve in order to accommodate ever-increasing instantaneous luminosities provides a unique opportunity for the development of novel DCS and DAQ systems. Once such emerging technology that has the ability to bring about a great shift in detector design is referred to as the Internet-of-Things (IoT). IoT can be defined as wireless communication amongst various devices (sensors) as well as an external network. The technology has broad applications to current and future detectors associated with the Large Hadron Collider and Future Circular Collider e-e+. The Wits Institute for Collider Particle Physics is undertaking a pilot project in order to develop the core skills required for the future development of IoT technology within particle detectors while also facilitating technology transfer. This project involves creating an air quality monitoring system comprising a mesh network of individual sensor nodes. The sensor array samples numerous air quality metrics and transmits them to a cloud for offline processing. An overview of the project will be provided with an IoT use case within particle detectors being discussed and will culminate in the presentation of the pilot
project.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics for Development, Education and Outreach / 204

Educational device for Electrochemical Impedance Spectroscopy

Author: Marco Mariola[1]

Co-authors: Senzo Hlongwane [2]; Petruccione Francesco [3]

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Electrochemical impedance spectroscopy is a method to investigate the properties of materials. The technique consists of sending an electrical stimulus into the material or solution, through two electrodes, and simultaneously measuring the impedance of the substance by varying the frequency. Once the impedance characterization is performed, the data are used to find the equivalent electric circuit of the examined material. In this work, an alternative device to commercial equipment is presented, in order to make it available to students for laboratory activities. The teaching-oriented project does not claim to create more precise and performing instruments available on the market. Still, the project aims to familiarize the student with the field of study.

Apply to be considered for a student ; award (Yes / No)?:

N

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 2 / 205

Characterization of Natural Polymeric Fibres with Resonance Acoustic Spectroscopy

Author: Sekhants'o Lara[1]

Co-author: Naleli Matjelo [2]

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Natural polymers are now being considered for composite materials because of their biodegradability in comparison to synthetic polymers. Hence much of scientific research is directed toward unleashing unknown and technologically applicable properties of these organically derived materials. Resonance acoustic spectroscopy uses sound waves as a probing medium to trigger vibrations of an elastic object. In this project, the resonance acoustic spectrometer was designed and constructed using portable radio speakers, a signal generator and a spectrum analyser. Natural polymeric fibres, disposed of as solid waste from the industrial extraction process of organic oils from rosehip (Rosa Canina), were then characterized for size, shape and composition. The preliminary results show some promising behaviour and more probing is currently underway.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Nuclear, Particle and Radiation Physics / **206**

Building a Hybrid Compton Camera System for Improving Proton Therapy Imaging

Authors: Shanyn Hart[1]; Stephen Peterson[2]; Luna Pellegri[3]; Pete Jones[None]

[1] *University of Cape Town and iThemba LABS*

[2] *University of Cape Town*

[3] *University of Witwatersrand and iThemba LABs*

Corresponding Author: hrtsha014@myuct.ac.za

The UCT POLARIS system, a solid-state CZT detector for prompt gamma-ray imaging, has shown potential for improving range verification techniques in proton therapy [1]. However, its limitations in timing resolution and energy range impede its clinical applicability. In this project, we aim to overcome these limitations by combining the POLARIS detector with a fast-timing 2" x 2" LaBr3$_3$(Ce) detector as a hybrid Compton camera [2] [3]. The LaBr$_3$(Ce) detectors have outstanding timing and energy resolution, and a higher maximum energy range, while the POLARIS detectors have high position sensitivity and excellent energy resolution. To investigate the feasibility of the hybrid setup, a pulse selected 66 MeV proton beam experiment was conducted at iThemba LABS.
The accurate tracking of double scatter gamma ray events from a POLARIS detector into a LaBr$_3$(Ce) detector requires careful coordination between the two systems. The onboard electronics of the POLARIS detector enable the selection of single scatter events within the CZT crystals. For background reduction, a cyclotron beam radiofrequency time of flight analysis is employed on the fast time data of the LaBr$_3$(Ce) detector [4]. This analysis allows for the identification and selection of gamma-ray events originating from interactions between the proton beam and the target. Implementation of these data reduction techniques, along with the intricate time synchronization of the two detector data acquisition systems, facilitates the precise tracking of gamma rays across the two detectors.
This Compton camera work offers the potential to enhance range verification techniques and facilitate the development of a clinical prompt gamma-ray imaging system. The successful deployment of such a system would improve treatment efficacy and bolster the role of proton therapy in cancer treatment.

References
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[2] Msebi L et al., *Nucl. Instrum. Methods. Phys. Res. B* **1026** (2022) 166195.
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Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / **207**

Using NLP to predict Alert Signals from the ATLAS TileCal Detector Control System at CERN

Author: Nicholas Perikli[None]

Co-authors: Edward Nkadimeng [1]; Bruce Mellado [2]

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[2] *University of the Witwatersrand and iThemba LABS, National Research Foundation*

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Using NLP to predict Alert Signals from the ATLAS TileCal Detector Control System at CERN

Nicholas Perikli on behalf of Tile Calorimeter Systems Team.
School of Physics and Institute for Collider Particle Physics, University of the Witwatersrand, Johannesburg, South Africa

Particle physics data consists of patterns in measurements that can be separated into hot topics and more mundane data. This approach is analogous to looking for keywords or topics in huge text data by separating more specific words and phrases from the generalities of text through the application of NLP. This will be done using the TileCal DCS alarm data of the ATLAS experiment. The NLP models that were constructed or fine-tuned for text classification included SVM, BERT- basecased, RoBERTa-base, as well as stacked LSTM and bi-LSTM. This was done on Google Colab using Pytorch and Python libraries, and the hyperparameters were optimised using the WandB platform, in which an extensive Baye's optimisation search was performed. The idea is to use the bestperforming models i.e., BERT or RoBERTa and train them by fine-tuning their hyperparameters in order to classify the alarms, as well as predict future alarm signals, and then follow the same procedure for an LSTM model and compare the results. The inputs would contain information about the date and time the alarm was received, the physical variable involved, the type of error as well as the particular system, component or sub- component affected.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / 208

Mechanism of lithium and magnesium oxides (LixOx and MgxOx) adsorption onto pristine graphene: Density functional theory approach

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Co-authors: M TIBANE ; R MAPHANGA

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We computationally investigated the adsorption behaviour of lithium oxides (LixOx) and magnesium oxides (MgxOx) onto pristine graphene during oxygen reduction reaction (ORR) for lithium air batteries operation using density functional theory (DFT). We proposed various pathways and studied different adsorption configurations in each system, comprising the O2, Li, and Mg as ORR reactants and the LiO2, MgO2, Li2O2 and Mg2O2 as ORR products. Mg atom weakly adsorbed onto graphene with an adsorption energy of (-0.035 eV to -0.043 eV), followed by O2 molecule (-0.101 eV to -0.134 eV) moreover Li atom adsorbed strongly with an adsorption energy of (-0.985 eV to -1.296 eV). The ORR product MgO2 adsorbed strongly with an adsorption energy of(-1.536 eV) than other reaction products LiO2, Li2O2 and Mg2O2 with their calculated adsorption energies of (+0.768 eV, -0.535 eV and -0.879 eV) respectively onto graphene. lastly the electronic properties (TDOS and PDOS) were calculated to understand their electronic behaviour.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics of Condensed Matter and Materials Track 1 / 209

Atomistic simulation studies of LixTiO2, NaxTiO2 and MgxTiO2 (x=0.11,0.15,0.19 and 0.23) nanosphere for metal ion batteries: Beyond lithium-ion Batteries.

Authors: Blessing Rikhotso[1]; P.E Ngoepe[1]; D.C Sayle[2]

[1] *University of Limpopo*

[2] *University of Kent*

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The demand of lithium rapidly increases year by year, pushing up the price and making lithium resources less affordable. Thus, it is crucial to find alternative technology beyond lithium-ion batteries (LIBs) that employs abundant elements on earth. Sodium (Na+) and magnesium (Mg2+) are suitable candidates due to their high abundance and low cost, as well as their compatible redox potential to lithium [1]. Generated TiO2 nanosphere architectured [2] are very promising as anode electrode materials for rechargeable batteries due to their ability to host more single (Li+ and Na+) and divalent (Mg2+) ions under highly extreme temperature conditions. In these studies, the simulation recrystallization of the LixTiO2, NaxTiO2 and MgxTiO2 nanosphere with x = 0.11,0.15,0.19 and 0.23 was atomistically synthesized from an amorphous precursor through the large-scale classical molecular dynamics (MD) method using the DL_POLY code [3] to predict its structural stability at varied temperatures. Recrystallisation synthesis was then proceeded by the cooling process towards 0 K; the cooled LixTiO2, NaxTiO2 and MgxTiO2 nanosphere structures were then heated from 100 K to 2000 K at temperature intervals of 100 K using an NVT Nose Hoover ensemble (exothermic reaction). The calculated correlation of the Ti - O pair was evaluated by their Radial Distribution Functions (RDFs), where the extent of crystallization was confirmed mostly after cooling synthesis. The simulated X-ray diffraction (XRDs) spectra agreed well with the experimental XRD's of pure TiO2 polymorphs [4], as well with the modelled respective microstructural defects, which all exhibited peak domains patterns of brookite (zigzag tunnels), anatase (complex tunnels) and rutile (straight tunnels) at all varied temperatures and Li+, Na+ and Mg2+ concentrations which are good properties for enhancing structural phase stability and energy storage capabilities. The Li+ and Na+ diffusivity rates within the TiO2 nanosphere both indicated a rapid increase in diffusion coefficients, Li+ had the highest diffusion coefficients more than that of Na+ and Mg2+ at all varied temperature and varied ion concentration. However, the sudden drop in Li and Na diffusivity rates on Li0.19TiO2 and Na0.19TiO2 nanosphere structures was due to the highly amorphous atom connectivity formed after all simulation synthesis. Furthermore, Mg2+ had a constant zero diffusion coefficients at all increased temperatures and ion concentrations within the TiO2 nanosphere. These results provide substantial new improvements and insights that LixTiO2, NaxTiO2 and MgxTiO2 nanosphere structures are an excellent candidate as anode electrode materials for lithium ions batteries (LIBs), sodium ions batteries (NaIBs) and magnesium ions batteries (MgIBs), due to their capabilities of storing more Li, Na and Mg atoms and withstanding highly extreme temperatures conditions while maintaining their structural phase stability and atom ordering to improve the battery performance.

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[4] B. N. Rikhotso, M.G. Matshaba, D.C. Sayle, P.E. Ngoepe, Optic. Mat.,102 (2020) 109831.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics of Condensed Matter and Materials Track 1 / 210

Derivation of empirical interatomic potentials for interactions that emanate from doping Li-Mn-O spinel with nickel and cobalt.

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Co-authors: Raesibe Sylvia Ledwaba [2]; Phuti Ngoepe [2]

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Molecular dynamics (MD) simulations which generally rely on empirically parameterized functions are currently the only practical option for large-scale computational studies of materials. The process of determining these parameters is quite a challenge, particularly given that the final potential parameters are extensively dependent on the initial parameters. Hence, finding initial parameters that are linked to the physical characteristics of the interaction is pivotal to the process, as such, we employ a machine-learning technique (to determine initial parameters) and the General Utility Lattice Program (GULP) (to determine final parameters) to develop accurate Buckingham interatomic potentials for interactions that arise from doping Li-Mn-O spinel with Co or Ni. The potentials will enable the correlation of various properties linked to the electrochemical performance of the Li-M-O spinel (M = Mn, Co, Ni) cathode materials to their microstructural changes through large-scale MD simulations. The exploration will provide insights on how to curtail the reported capacity fading of Li-Mn-O spinel which is a promising cathode material for lithium-ion batteries. A curve_fit function of the SciPy library was used to determine the initial potential parameters, which are thereafter refined with GULP. Moreover, the developed potentials are tested by performing MD simulations with the DL_POLY code. The final Buckingham potential parameters for all the interactions that arise from doping Li-Mn-O spinel with Ni and Co were successfully derived. The fitted and calculated lattice parameters were comparable with a percentage difference of less than 4 %. X-ray Diffraction (XRD) graphs of the simulated spinel structures (LiCo2O4, LiNi2O4, LiMn1.875Ni0.125O4, and LiMn1.875Co0.125O4) showed the presence of the LiM2O4 and M3O4 (M = Mn, Co, Ni) phases which are in line with findings in literature. The RDF graphs of the doped structures show that doping Li-Mn-O spinel with Co could enhance structural stability.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / 211

Low-budget atmospheric monitoring system.

Author: Marco Mariola[1]

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[2] *University of KwaZulu-Natal*

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General systems to monitor the atmospheric condition, such as humidity, temperature, and pollution are extensively used in research and also even for public health purposes. In terms of pollution, the atmospheric analysis can be performed by LIDAR, a local measuring station, or a ballon-based sensor.
The atmospheric sensor proposed aims to be a payload for a balloon or drone. As with other atmospheric sensors, the proposed system includes sensors, a Global Positioning System (GPS), and a radio transmitter to receive data about the position of the station and the data collected by the sensors. The aim of the project is to be a system that is easy to modify and to be able to be adapted to the research needs. For this purpose, the system is entirely based on open-source electronics, except for some sensitive parts, such as the transmitter.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Consent on use of personal information: Abstract Submission:

Applied Physics / 212

Computational fluid dynamics modelling of airborne droplets

Authors: Mbolahasina Ralijaona[1]; Emmanuel Igumbor[1]; Kennedy Otwombe[2]; Firdaus Nabeemeeah[3]; Neil Martinson[3]; Minja Milovanovich[3]; Pedro Mafa[4]; Lerothodi Leeuw[5]; Simon Connell[1]

[1] *Department of Mechanical Engineering Science, University of Johannesburg, Auckland Park, Johannesburg, South Africa*

[2] *Perinatal HIV Research Unit, Chris Hani Baragwanath Academic Hospital, Faculty of Health Sciences, University of the Witwatersrand South Africa School of Public Health, Faculty of Health Sciences, University of the Witwatersrand South Africa*

[3] *Perinatal HIV Research Unit, Chris Hani Baragwanath Academic Hospital, Faculty of Health Sciences, University of the Witwatersrand South Africa*

[4] *Department of Mathematical Sciences and UNISA - ATLAS High Energy Physics Group, University of South Africa, Johannesburg, 1710, South Africa*

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Corresponding Author: ralijaonahasina@gmail.com

Airborne transmitted diseases are a public health concern. They are ubiquitous in human's life and include large variety of diseases such as the common cold, chicken pox, mumps and more serious ones like COVID-19 and tuberculosis. The aforementioned diseases are transmitted through saliva droplets emitted in the environing air. While being airborne, droplets are affected by multiple environmental factors mainly air flow, humidity, and temperature. Furthermore, droplets are interacting with the surrounding air, exchanging mass and momentum. Droplets are also released under specific conditions defined by parameters like injection speed, the height from where they are emitted, their size distribution, and temperature. The physical processes involved in droplets' evolution over time have influence on how they are spread and likely to transmit pathogens. Thus, it is crucial to understand those processes for the purpose of attenuating transmission. This study focuses on modelling droplets' dispersion, evaporation, infectiousness with computational fluid dynamics (CFD). The two-way coupling approach was applied to compute momentum and mass exchange between droplets

and its environment. Interactions between particles were also considered with the stochastic collision model including droplet breakup and coalescence. The Rosin-Rammler distribution was used for the size distribution of droplets with a range varying from 1 to 200 μm. When increasing the speed at which droplets are ejected, particles are occupying a wider range of position, more spread and reaching farther distance. Increasing injection velocity is equivalent to considering different respiratory events from which particles are generated. In fact, speaking has a lower injection speed than coughing which injection velocity is lower than that of sneezing. Therefore, violent respiratory events are more likely to transmit diseases because droplets are more spread. Infectiousness of droplets are neutralized in a reasonable amount of time under the condition that evaporation is occurring. For the safety of public and confined spaces, it is encouraged to fulfil the conditions that trigger evaporation like aeration. Our model will be used as a guide for configuring clinical and public spaces.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 1 / **213**

Strain Evolution with Thickness of TbMnO3/ (001) SrTiO3-TiO2 term. Epitaxially-strained Thin Films

Author: Geoffrey Mwendwa[1]

Co-authors: Daniel Wamwangi [1]; Lesias Kotane [1]; Rudolph Erasmus [1]; Milani Radović [2]; Hugo Dil [3]; Dave Billing [4]; Adam Shnier [4]; Morgan Madhuku [5]

[1] *School of Physics, Material Physics Research Institute, University of the Witwatersrand, Johannesburg, South Africa*

[2] *Photon Science Division, Paul Scherrer Institute, Villigen, Switzerland*

[3] *Institut de Physique, École Polytechnique Fédérale de Lausanne, Switzerland*

[4] *School of Chemistry, Molecular Sciences Institute, University of the Witwatersrand, Johannesburg, South Africa*

[5] *iThemba LABS (Gauteng), Johannesburg, South Africa*

Corresponding Author: geofmutua@gmail.com

Strain in multiferroic rare-earth epitaxial layers is a key feature that can induce new functionalities for the next generational applications such as room-temperature magnetoelectricity and magnetocapacitance [1, 2]. Several studies have shown the modulation of strain in TbMnO3 (TMO) thin films as a promising route for fabrication of perovskite-type oxides with tunable electrical and magnetic properties.

This work explores the evolution of strain in TMO thin films grown epitaxially on (001) SrTiO3-TiO2 term. single crystal substrates using ultra-high vacuum pulsed laser deposition technique. In-situ monitoring of the film growth by using reflective high-energy electron diffraction (RHEED) have shown the formation of Kikuchi lines which verified the film orientation in (001) for the TiO2 terminated SrTiO3 substrate. The film quality and variation of strain as a function of thickness were investigated using X-ray diffraction and X-ray reflectivity. A rocking curve of the (002) peak further confirms the high crystalline quality of the films. Further analysis of the X-ray diffraction patterns confirm successful growth of single-phase c-axis-oriented epitaxial TMO films with an orthorhombic structure. Quantitative strain analysis has shown reduction of strain with increasing thickness.

Keywords: Multiferroic, perovskite, epitaxial growth

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[1] G. Panomsuwan and N. Sait, *Cryst. Res. Technol.* 2018, 53, 1700211
[2] V. Goian *et al, COMMUNICATIONS MATERIALS*, (2020) 1:74

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / **214**

Measurement and simulation of secondary neutron production from a 66 MeV proton beam

Author: Josiah De Klerk[1]

Co-authors: Andy Buffler [2]; Stephen Peterson [2]; Tanya Hutton [2]

[1] *University of Cape Town Physics department*

[2] *University of Cape Town*

Corresponding Author: josiahchristiandeklerk@gmail.com

Prompt gamma rays (PGs) produced by nuclear collisions during proton therapy (PT) can be used for *in vivo* proton beam range verification through a technique known as prompt gamma imaging (PGI). During PT, the production of PGs within the tissue provides a reliable location map for the proton dose deposition. The detection of these PGs using a Compton Camera (CC) can be used to construct a source image of the PGs. Since the reconstructed source image is dependent on the quality of the detection, the detection efficiency of a CC device can be negatively affected by additional secondary radiation (particularly neutrons) produced alongside the prompt gamma rays. The goal of this work is to understand the characteristics of these secondary neutrons during a proton beam irradiation and their potential impact on a CC.
The experimental setup consisted of a 66 MeV pencil beam of protons on a variety of targets (HDPE, water, graphite) with the neutron measurements made using an organic liquid scintillator detector (BC-501A) at several angles within the K600 vault (S-line) at iThemba LABS. To obtain neutron energy spectra with the BC-501A an unfolding procedure is typically used, where energy spectra are deconvolved from the measured, and calibrated, neutron light output spectra. As the quality of the unfolding is dependent on the prior knowledge of the energy spectrum, a Geant4 simulation was constructed to better understand the produced neutron field and aid the unfolding process. A comparison of the experimental and simulated results will be discussed.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Nuclear, Particle and Radiation Physics / **215**

Determination of reaction activities on Au and Tm targets using the quasi-monoenergetic neutron beams at approximately 90 MeV

Author: Luyanda Ndevu[1]

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Determination of reaction activities on Au and Tm targets using the quasi-monoenergetic neutron beams at approximately 90 MeV
Ndevu L1,2, Lethole NL1, and Maleka PP2
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The International Atomic Energy Agency (IAEA) has highlighted the challenge of managing highly radioactive waste from nuclear reactions, and one potential solution being considered is the use of accelerator-driven sub-critical systems (ADS) [1]. However, constructing such reactors requires experimental neutron cross-section libraries for (n, xn) reactions in various materials at energies above 20 MeV, which currently are scarce or have large uncertainties [2]. To address this gap, this study aims to perform preliminary measurements on the reaction product activities of 197Au and 169Tm target materials using quasi-monoenergetic neutron beams of approximately 90 MeV. The study utilized the iThemba LABS neutron beam facility to produce quasi-monoenergetic neutron beams. Neutron detectors were used on the 0° and 16° beam paths to obtain spectra, which were then compared to determine the neutron flux. Stacked target materials including 197Au and 169Tm were irradiated and also placed along the 0° and 16° beam path. Neutron detectors and target materials were placed at least 5 m from the Li target, the neutron production point.
After irradiations, the samples were counted on a gamma-ray counting system to identify the reaction products and calculate the activities of the identified nuclei. The experimental procedure used to determine energy and efficiency calibrations with the gamma-ray spectrometry method will be discussed during the presentation. The results of this study are expected to contribute to the improvement of the International Reactor Dosimetry and Fusion File (IRDFF) library [3] and provide a benchmark for validating nuclear models and improving nuclear data libraries.

[1] Bielewicz et al., The New Collaboration of the JINR and the iThemba LABS for Cross-Section (n,xn) Reactions Measurements (2019).
[2] Pomp et al., Radiat. Prot. Dosimetry 161 (1-4), 62–66 (2014).
[3] Trkov et al., Special issue of Nucl. Data Sheets, 163, 1-108 (2020).

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / 216

Influence of pyrolysis temperature on the mesoporous graphitic carbon nitride and its effect on physicochemical properties for energy application.

Author: Tshegofatso Memory Modungwe[1]

Co-authors: Guy Leba Kabongo [1]; Simon Dhlamini [1]; Pontsho Mbule [1]

[1] *University of South Africa*

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Graphic carbon nitride (GCN) was synthesized through a direct pyrolysis of urea at different calcination temperatures (450,500, 550, and 600 ℃). The effect of the pyrolysis temperatures on the structural, compositional, morphological, and surface area properties were studied. The GCN powders were characterized through X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Field emission scanning electron microscopy (SEM), and Brunauer-Emmett-Teller (BET). The XRD analysis showed that the samples consist of two characteristic reflections (100) and (002) belonging to graphitic carbon nitride. A close examination at the (002) peaks uncovers that as the calcination temperature rises the peak slightly shifts towards a higher 2 theta diffraction angle. This leads to the deduction that increasing the pyrolysis temperature can improve the interlayer stacking order of g-C3N4. The crystallite sizes were determined by the Debye-Scherer method and found to increase with pyrolysis temperature. The FE-SEM images revealed that there is variation in the surface morphology of the samples depending on the calcination temperature. The FTIR confirmed the presence of functional groups and chemical bonds. Finally, the BET showed that the samples were mesoporous with pore sizes ranging from 2- 20 nm. The specific surface area was 32.31, 37.14, 56,64, and 51.59 m2/g for 450, 500, 550, and 600 ℃ respectively.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics of Condensed Matter and Materials Track 2 / 217

Tin Oxide nanoparticle structural modification with ZnO/Zn for gas sensing applications.

Author: Philani S. Mngomezuulu[1]

Co-authors: Charles T. Thethwayo [1]; Puleng N. Biyela [1]

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Tin oxide nanoparticles were synthesized using hydrothermal process, tin tetrachloride was dissolved in distilled water, and ammonia was used as a precursor to control pH. Zinc and zinc oxide were used as dopants to modify the structural properties of tin oxide nanoparticles. The synthesized nanoparticles were characterized using the X-ray diffraction (XRD), high resolution transmission electron microscope (HRTEM), scanning electron microscope (SEM), and X-ray photoelectron microscope (XPS) to study their structural, morphological, average particle size and surface properties.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Nuclear, Particle and Radiation Physics / 218

39Ca and its relevance in nuclear astrophysics

Author: Sifundo Binda[1]

Co-authors: Lindsay Donaldson [2]; Luna Pellegri [3]; Philip Adsley [4]

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[2] *iThemba Laboratory for Accelerator Based Sciences*

[3] *University of Witwatersrand and iThemba LABs*

[4] *Cyclotron Institute, Texas A&M university / Department of Physics and Astronomy, Texa A&M university*

Corresponding Author: sifundobinda1@gmail.com

Elemental abundances are excellent probes of classical novae (CN). Sensitivity studies show that ^{38}K(p,γ)^{39}Ca reaction rate uncertainties modify the abundance of Ca by a factor of 60 in CN ejecta. Direct measurements of the ^{38}K(p,γ)^{39}Ca reaction have reduced the uncertainties but discrepancies in resonance energies between different experiments persist. To resolve these, ^{39}Ca was studied using the ^{40}Ca(p, d)^{39}Ca reaction at a beam energy of 66 MeV using the K600 magnetic spectrometer. This will verify the properties of levels in the region where discrepancies between experiments persist. Preliminary results from the measurements will be presented.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics for Development, Education and Outreach / **219**

Vectors in Physics: Challenges for First-Year University Entering Students

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Physics education covers various topics, including classical mechanics, electromagnetism, thermodynamics, quantum mechanics, and relativity. In most topics in physics, vectors are essential because they represent physical quantities such as displacement, velocity, acceleration, force, and momentum. These quantities have both a magnitude and a direction, and vectors provide a convenient way to represent them mathematically. In summary, vectors are essential in mathematics, science, engineering, and technology. They provide a way to express and manipulate complex physical and mathematical quantities and are used in various applications. Teaching about vectors in the first year includes theoretical and practical aspects. It aims to equip learners with the mathematical and scientific skills necessary for higher levels and career paths. This paper investigates how first-year physics students deal with vector problems in physics. The study formally assessed over 200 students, focusing on vector concepts to explore the challenges students face in answering questions, intending to equip first-year students with the right skills to solve vector problems. The study aimed to investigate the conceptual difficulties that the First year entering students have in understanding vector concepts. The results show that most students need help understanding vectors in physics. The study has highlighted the areas where these students need help understanding vectors.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Astrophysics & Space Science / **220**

Searching for pulsars and FRBs in an extragalactic source with MeerKAT

Authors: Heinrich Hurter[None]; Christo Venter[1]; Anu Kundu[2]; Benjamin Stappers[3]; Lina Levin Preston[3]

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Pulsars, the aftermath of core-collapse supernovae, rotate rapidly and have immense magnetic fields. These characteristics lead to broad-band radio emission. The radio pulses are believed to be emitted above the pulsar's magnetic polar caps. The MeerKAT radio telescope, which is situated in Carnarvon in the Northern Cape, South Africa, is ideally suited to discover new pulsars due to it being located in a radio-quiet area with minimal radio interference, and its excellent sensitivity. Our project is part of the Transient and Pulsars with MeerKAT (TRAPUM) survey project, which aims to discover new pulsars and transient events. We investigated seven potential extragalactic sources, focusing on their stellar population, star-formation rates, and masses. We then chose the most promising galaxy (NGC253) for observation by MeerKAT. An upper limit has been set on pulsar emission from this galaxy. We will discuss the selection criteria, search methods, upper limit, and future prospects in this presentation.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Applied Physics / **221**

A computational fluid dynamics study of the infectiousness decay of SARS-CoV-2 microorganism when exposed to UVGI combined with evaporation

Authors: Emmanuel Igumbor[1]; Mbolahasina Ralijaona[2]; Pedro Mafa[3]; Lerothodi Leeuw[4]; Simon Connell[1]; Kennedy Otwombe[5]; Neil Martinson[6]; Firdaus Nabeemeeah[6]

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Respiratory diseases propagated by droplet-based transmission are serious public health hazard, leading to pandemics, such as the Coronavirus outbreak. One engineering intervention used to mitigate the spread of droplet-based transmission pathogens is ultraviolet germicidal irradiance (UVGI). The UVGI device is able to disinfect air and surfaces through intense ultraviolet germicidal irradiance, which damages infectious microorganisms. This process coupled with environmental conditions such as evaporation helps to reduce the spread of aerosol transmission of pathogens. Despite tremendous research progress on mitigation of the spread of infectious diseases reported, there is no adequate information on the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) infectiousness decay when exposed to UVGI combined with evaporation process. In this study a computational fluid dynamics (CFD) simulation with the combination of parameters describing the UVGI intensity field, humidity, temperature and relative motion (droplet and fluid) was used to investigate the infectiousness decay of SARS-CoV-2 in a confined room. Droplets propagating SARS-CoV-2 were tracked using the discrete phase model as implemented in ANSYS-FLUENT. Augmentation of the standard models were developed as using an external scalar to track infectiousness via a user define function so as to determine the survival rate and the infectiousness decay of droplets propagating SARS-CoV-2 at specific relative humidity and temperature values, during coughing, speaking, and sneezing of a carrier in a confined room. The infectiousness of SARS-CoV-2 significantly reduced when exposed to UVGI coupled evaporation. Therefore, we suggest that the spread of the infectiousness of SARS-CoV-2 in a confined room can be investigated using our proposed model. Furthermore, we show that our model can be used to optimize engineering interventions, thus forming the basis of understanding and controlling infectiousness of droplets propagating SARS-CoV-2 in a confined public health space. In the future, our model proposed in this study can be extended to mitigate the spread of other infectious airborne diseases in public schools, clinics, and transport systems

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

No

Nuclear, Particle and Radiation Physics / **222**

Photon Strength Function Measurements at iThemba LABS

Author: Kgashane Malatji[1]

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The study of statistical nuclear properties is of importance not only in nuclear waste transmutation [Colonna2010] and nuclear fuel cycles [Report2006] but also in nuclear structure and nuclear astrophysics studies [Arnould2003]. These statistical properties - the nuclear level density (NLD), which describes the number of available energy levels in a nucleus for a given excitation energy, and the photon strength function (γSF), which is the electromagnetic decay probability for a nucleus to either emit or absorb a gamma-ray, are critical ingredients into calculations of neutron capture cross sections and astrophysical reaction rates.

This presentation will discuss measurements of nuclear level densities and photon strength functions performed at iThemba LABS and their applications.

[Colonna2010] N. Colonna et al., Energy Environ. Sci. 3, (2010) 1910.
[Report2006] Report of the Nuclear Physics and Related Computational Science R\&D for Advanced Fuel CyclesWorkshop, DOE Offices of Nuclear Physics and Advanced Scientific Computing Research (2006).
[Arnould2003] M. Arnould and S. Goriely, Phys. Rep. 384 (2003) 1–84.

This work is based on the research supported by the National Research Foundation of South Africa Grant Number 118846.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Nuclear, Particle and Radiation Physics / **223**

Growing evidence of new scalar at the large hadron collider with a mass around 152 GeV

Authors: Salah-eddine Dahbi[1]; Bruce Mellado[2]

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[2] *University of the Witwatersrand and iThemba LABS, National Research Foundation*

Corresponding Author: salah-eddine.dahbi@cern.ch

After the discovery of a Higgs boson at the Large Hadron Collider (LHC) by the ATLAS and CMS experiments, a number of multi-lepton anomalies that represent a significant experimental evidence for a new physics have been identified. These anomalies are consistent with the decay of a heavy boson H with a mass around 270 GeV, into a Higgs like boson S of a mass around 150 GeV. The latter can be inferred from the invariant mass of final states with opposite sign leptons in these multi-lepton excesses. Motivated by this indirect evidence of a beyond the standard model of particle physics (BSM) scalar, we performed a combined fit of several direct searches for a Higgs-like by ATLAS and CMS, within the mass region of the S scalar. The results of this combination are compared with predictions for a resonant pair production of the S in a simplified model. A local significance of 5.2 σ is achieved for a mass of $m_S = 152$ GeV. This therefore indicates a more stringent evidences for a new scalar at 152 GeV, in multiple decay channels, such as, $Z\gamma$, $\gamma\gamma$, WW, $e\mu$ final states.

Apply to be considered for a student ; award (Yes / No)?:

no

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Applied Physics / **224**

Modelling Weather Patterns and Solar PV systems for the Sizing of Standalone PV Battery Charging System Standalone PV Battery Charging System

Author: Happy Sibusiso Ndlovu[None]

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Introduction

However, designing an effective and efficient PV battery charging system requires careful consideration of several factors, including the weather patterns of the region.
Specifically, we focus on modeling the weather patterns of the region and the performance of the PV system under those conditions in order to identify the most suitable system configuration for reliable and efficient battery charging.
The study must develop a comprehensive model that can accurately predict the solar resource availability and energy production potential of the system, considering the variability of weather patterns and the performance characteristics of the PV panels and battery system.

Methodology

To investigate the use of weather patterns and PV system models for the sizing of standalone PV battery charging systems, we conducted a simulation-based study using weather data and PV system models for a rural region.
1. The historical weather data for the region collected, including variables such as temperature, solar irradiance, wind speed, and precipitation. We then used this data to develop a statistical model of the weather patterns for the region, including seasonal and daily variations.

Next, We will then use the weather and PV system models to simulate the performance of various system configurations for battery charging, including different panel sizes, battery capacities, and charge controller settings.
We will evaluate the performance of each configuration based on factors such as battery charge time, energy efficiency, and system reliability.
Finally, we will compare the performance of different system configurations and identify the optimal configuration for the given weather patterns and system requirements. Our results will provide insights into the use of weather data and PV system models for the design and optimization of standalone PV battery charging systems for Northern KwaZulu-Natal.

Result

The following figure showing the out of the Modell I already trained for the meteorological data, which shows the model is not performing well:

Whereby recall is a metric that measures the ability of a model to identify all relevant instances of a particular class or label in a dataset. Precision is a metric that measures the ability of a model to identify positive predictions correctly. The F1 score is a measure of a machine learning model's accuracy that considers both precision and recall. Accuracy is the measure of the model to do the right prediction.

Discussion

This study focused on the use of weather modeling techniques and solar PV system simulations to determine the optimal sizing of standalone PV battery charging systems for rural areas. The results highlighted the importance of accurately modeling both weather patterns and solar PV system performance in order to design an effective system. Cloud technologies such as Azure ML and Amazon SageMaker will be used to improve the accuracy of the model. The study has important implications for the design and implementation of standalone PV battery charging systems in rural areas, helping to bring reliable and sustainable energy solutions to rural areas.

Conclusion

In this study, we have demonstrated the effectiveness of using weather pattern modeling in conjunction with solar PV system modeling to accurately size standalone PV battery charging systems for rural areas. By accurately sizing standalone PV battery charging systems, we can ensure that rural communities have access to reliable and sustainable energy sources that can improve their quality of life.

Apply to be considered for a student ; award (Yes / No)?:

YES

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Consent on use of personal information: Abstract Submission:

Theoretical and Computational Physics / **225**

Quantum Field Theories in Finite Systems

Authors: William Horowitz[1]; Jean Du Plessis[1]

[1] *University of Cape Town*

Corresponding Author: dpljea028@myuct.ac.za

We are interested in the effect of finite system size corrections to the QCD equation of state in heavy-ion collisions, to better understand the apparent formation of Quark Gluon Plasma in proton-nucleus and even proton-proton collisions. To do so, we need to build up the necessary understanding of Quantum Field Theories(QFTs) in finite systems.

To this end we derived for the first time the finite system size corrections to NLO $2 \to 2$ scattering in a scalar toy model (massive ϕ^4 theory). In order to aid in this derivation we needed to develop multiple novel techniques, including denominator regularization, and an analytic continuation of the generalized Epstein Zeta function, and a direct generalization of a formula originally proposed by Ramanujan.

In this talk I discuss this derivation and more importantly the techniques developed, which we expect to be useful in the further study of finite system size corrections to QFTs. I will further discuss the numerical results for the derived scattering amplitude, as well as what it means for future investigations, including some observations about geometry-induced bound states.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / **226**

2D/3D heterojunction of MAPbI3/OA2PbI4 thin films for Photovoltaic Hydrogen Evolution

Author: Sandile Thubane[None]

Co-author: Mmantsae Diale [1]

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Three-dimensional (3D) halide perovskites have emerged as a promising class of inexpensive and easy-to-make semiconductors for photocatalytic application in hydrogen evolution due to their exceptional visible light response. Their high sensitivity to humidity, however, resulted in significant instability issues. This led to the development of 2D/3D halide perovskites (HaP), which showed

efficient charge-carrier transport, humidity resistance, and higher stability in ambient conditions. In this study, a pure 3D MAPbI3, 2D OA2PbI4, and 2D/3D OAxMA1−xPbI3 HaP were synthesized using the spin-coating method. From the X-ray diffraction (XRD) results, a 3D HaP was confirmed at 14.1° and 28.4°, whilst a 2D HaP depicted its characteristic peaks in the low 2θ area at 5.5°. Also, the 2D/3D HaP powder shows identifiable reflections assigned to the OA2PbI4. The morphological studies of the 2D, 3D, and 2D/3D powders were studied using a scanning electron microscope (SEM). The HaP materials exhibit particle sizes of 100 nm for 3D, 400 nm for 2D, and around 200 nm for 2D/3D HaP with mixed phases. The pristine 3D nanoparticles with clear grain boundaries have relatively different appearances, while the 2D/3D particles with different cation ratios all show good crystallinity as confirmed by XRD. In contrast to the MAPbI3, which exhibits a significant absorption over the entire visible range, the OA2PbI4 exhibits a major absorption peak in the UV spectrum at 375 nm, which is above the visible range. Furthermore, the 2D/3D displays a longer onset than the pristine 3D HaP and similar strong visible light absorption across the entire visible range. Pure 2D perovskite exhibits the lowest photocatalytic hydrogen evolution (PHE) rate of 192.1 mol g-1 h-1 while the pristine perovskite exhibits a PHE rate of 323 mol g-1 h-1 within 5 hours. The PHE rates are, however, 219.3, 430.2, 960.2, and 274.5 mol g-1 h-1 for the 2D/3D HaP with octadecylamine (OA) concentrations of 5, 10, 15, and 25%, respectively. The outcomes show that the 2D/3D perovskite with the ideal OA content of 15% had the best performance. The 2D/3D HaP show the same characteristic peaks before and after the PHE, indicating a high stability of the materials. The transient photocurrent responses (i-t curves) and electrochemical impedance spectroscopy (EIS) of the perovskites coated on fluorine-doped tin oxide (FTO) were performed under illumination with a single wavelength of light at 420 nm. The results showed that the OA0.15MA0.85PbI3 exhibits the strongest photocurrent, indicating the most effective electron-hole separation and transportation.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Theoretical and Computational Physics / **227**

Deep Inelastic Scattering in Nuclear Collisions

Author: William Horowitz[1]

[1] *University of Cape Town*

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Deep inelastic scattering (DIS) is a key measurement in nuclear physics. One of the massive advantages of DIS is that powerful mathematical theorems–known as factorization–have been proven. We discuss the application of these theorems and effective field theory to collisions between electrons and protons and the potential extension of these theorems to collisions between electrons and nuclei, which will be relevant at the future eRHIC facility.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / **228**

The structural, electronic and dynamical properties of pyrite-type minerals: DFT and Atomistic Simulations.

Author: Mofuti Mehlape[1]

Co-authors: Kgwajana Barnard Molala [2]; Phuti Ngoepe [2]

[1] *University Of Limpopo*

[2] *University of Limpopo*

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Pyrite is the most common sulphide gangue mineral occurring in base metal sulphide ores around the world. FeS2 is one of the most commonly occurring metal sulphide minerals. Despite its low economic value, its properties have been explored extensively over the years. However, the study of properties of other pyrite-type minerals are still lacking. This work use computational modelling simulation methods to examine the properties of the pyrite-type minerals (MS2, where M = Co, Ni), that have a similar chemical composition. The work will be conducted through the derivation of interatomic potentials. Density Functional Theory (DFT) method was used to calculate the structure and elastic properties of pyrite-type minerals. Subsequently, the DFT data was used for the derivation of interatomic potentials for atomistic simulation. The constructed interatomic potentials were validated by subjecting the minerals to extreme conditions, i.e. temperatures and pressure through molecular dynamics simulations. The structure and elastic properties are in qualitative agreement with DFT data and those from literature. Furthermore, the potentials will be useful into the fundamental understanding of the collectors and surface interaction mechanisms involved in mineral processing.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 1 / 229

Preparation of highly sensitive Cr doped ZnFe2O4 fiber-like sensors for selective acetone detection

Author: Murendeni Nemufulwi[1]

Co-authors: Hendrik Swart [2]; Gugu Mhlongo [3]

[1] *University of free state*

[2] *UFS*

[3] *CSIR*

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Semiconducting metal oxides are widely recognized as key sensing materials that are used for gas detection in several fields. In particular, zinc ferrite has attracted growing attention because of its sensitivity to volatile organic compounds, making it a potential sensing material for food spoilage detection/monitoring [1]. However, the high operating temperatures and poor selectivity hinder practical application. This work aims to overcome these challenges by using Cr dopant to reduce the operating temperature and enhance the response variance for accurate gas classification using principal component analysis. A combustion method was used to synthesize Cr-doped ZnFe2O4 (0.0, 0.5, 1.0, and 1.5 Cr mol%) fiber-like products. XRD and HRTEM were used to analyse microstructure and morphology of the products. TEM confirmed that the morphology of the synthesized products possesses fiber-like structures. Optical properties of the products were studied using PL and XPS was

used for surface composition analysis. The gas sensing results showed that the sensor based on 1.0% Cr-doped ZnFe2O4 had an enhanced response of 283-90 ppm acetone at a low operating temperature of 90 ℃. Moreover, the sensor based on ZnFe2O4 doped with 1.0% Cr can be used as a single array sensor for gas classification. The improved sensing properties are attributed to structural defects and proper gas diffusion.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / 230

Performance evaluation of a 5kWp photovoltaic system in the Eastern Cape

Authors: Russel Mhundwa[1]; Michael Simon[2]

[1] *University of Fort Hare Institute of Technology*

[2] *FHIT*

Corresponding Author: rmhundwa@gmail.com

Most areas in South Africa receive an average more than 2 500 hours of sunshine per year, and average solar-radiation levels range between 4.5 and 6.5kWh/m2 in one day. This has necessitated the use of solar energy in South Africa, solar energy lends itself to several potential uses and the country's solar-equipment industry is developing. Residential homes have since started installing solar PV systems given the challenges that the country's energy supply. In this paper, the performance analysis of a standalone 5 kW solar system has been conducted. The system is installed on a residential home with a 5 kW hybrid inverter, 5 kWp PV modules, and a storage battery bank of 9 kWh for supplying the domestic load. The system was programmed to prioritize the load and excess used to charge the battery which was then used as a source of energy to compliment the PV during the day and in night-time used to supply electricity to the load. The system data was collected for a period of four months that is April to July 2022, and the variation of daily energy production, consumption and battery bank input or output energy were analyzed. The findings from this study enables understanding of hybrid inverter systems which will provide useful reference in the future applications of these inverters in the residential areas.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 1 / 231

The effects of chromium metal ion on belt-like In2O3 products and their ethanol gas sensing properties

Author: Mosima Kgomo[1]

Co-authors: Hendrick Swart [2]; Gugu Mhlongo [1]

[1] *CSIR*

[2] *University of Free State*

Corresponding Author: mosimakgomo@gmail.com

This study focuses on surface defect rich 1D fiber-like Cr-doped In2O3 products produced via electrospinning. The effects of Cr dopant ions on the ethanol gas sensing behaviour of the 1D fiber-like Cr-doped In2O3 products were examined. Explicit analysis pertaining to the structure, morphology, and surface related defects of the 1D fiber-like Cr-doped In2O3 products was conducted to obtain information on the gas sensing results. The Cr-doped In2O3 sensor with 1 mol% doping level presented improved gas sensing characteristics, exhibiting a reduced working temperature from 100 to 80 ℃, a high responsive value of 12, and rapid response/recovery times of 41/43s towards 50 ppm ethanol gas. A low detection limit of 2.18 ppm, as well as high selectivity and excellent stability towards 50 ppm of ethanol gas, was also demonstrated by this sensor. XPS analysis indicated that the improved gas sensing results stem from the maximum number of oxygen vacancies and chemisorbed oxygen species induced by the introduction of Cr dopant ion inside the In2O3 lattice. The high number of oxygen vacancies facilitated the adsorption of the ethanol gas molecules on the sensor material, while the large number of chemisorbed oxygen species permitted a high number of oxygen molecules to be chemically adsorbed on the sensor material.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 1 / 232

High selective and sensitive acetone gas sensor: Effects of Cerium metal ion on pyramid-like In2O3 products

Author: Mosima Kgomo[1]

Co-authors: Hendrick Swart [2]; Gugu Mhlongo [1]

[1] *CSIR*

[2] *University of Free State*

Corresponding Author: mosimakgomo@gmail.com

Herein, a high-performance acetone gas sensor based on pyramid-like Ce-doped In2O3 products was generated using a facile electrospinning approach followed by annealing at 550 ℃. Systematic characterization techniques demonstrated that the introduction of Ce dopant ions into the In2O3 lattice can improve the acetone gas sensing properties by inducing a high concentration of oxygen vacancies at different Ce dopant levels through the Ce3+/Ce4+ redox couple. A contrast of the acetone gas sensing performance of the pure and Ce-doped In2O3 sensors at doping levels of 0.5, 1.5 and 2 mol% showed that all Ce-doped In2O3 sensors exhibited high selectivity and high response towards 90 ppm of acetone at 150 ℃ with a 1.5 mol% Ce-doped In2O3 sensor presenting a maximum response value of 12, which is three-fold greater than that of the pure In2O3 sensor and a low detection limit of 1.98 ppm. With such enhanced acetone gas sensing capabilities, the Ce-doped In2O3 sensor with a doping level of 1.5 mol% can be utilised as an auspicious gas sensing layer for detecting acetone gas in real environments.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics of Condensed Matter and Materials Track 2 / 233

Structural, Mechanical and Electronic Properties of Lithium Nickel Oxide Bulk(LiNiO2) and Surface Stability

Author: Mmeshi Hiine[None]

Co-authors: Phuti Ngoepe [1]; khomotso Maenetja [2]

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Lithium-ion batteries have gained a lot of interest as a result of the increased demand for renewable energy sources, with LiNiO2 (monoclinic) being an ideal choice to be used as the cathode material. This is due to its high specific capacity (275 mAhg−1) and energy density (629 Whkg-1). However, LiNiO2 has low cycling stability and voltage fading, which restricts its usefulness. In this work we discuss the bulk structural properties using the First-Principle density functional theory and the low Miler index surfaces of LiNiO2 calculations were modelled using METADISE code. It was found that the lattice parameters are in good agreement with the reported results, with less than 1.5% difference and it have heats of formation of -624.37 kJ/mol which shows that our system is thermodynamically stable. Calculated elastic constants show that the structure is mechanically stable due to the agreement with the monoclinic stability criteria. Furthermore, the phonon dispersion curves show imaginary vibrations along the gamma region, indicating that the structures instability. LiNiO2 depicts an indirect bandgap of 0.00eV around the fermi-level suggesting that the structure has magnetic metal characteristic. Finally, we were able examine the following Miller index surfaces (i.e. (110), (100), (100), (010), (001), (111), and (101)), and found the most stable facet to be (101).

Keywords: Lithium-ion batteries, LiNiO2, Density functional theory(DFT),

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics of Condensed Matter and Materials Track 1 / 234

Multi-Faceted Approaches To Enhance The Li7La3Zr2O12 Solid Electrolyte Material

Author: Raesibe Ledwaba[1]

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Solid-state technology is by far the most intriguing development to curb the thermal instability associated with the reactivity of liquid electrolytes. Of particular interest is the cubic Li7La3Zr2O12 (LLZO) solid electrolyte material with ionic conductivity of 10−3 to 10−2 S•cm−1. However, it has temperature-dependent phase instability wherein the low conducting tetragonal phase exists below 630 ℃ whilst the highly conductive cubic phase is only stable at high temperatures. Herein, we explore several strategies incorporated in the fundamental enhancement of the LLZO solid electrolyte i.e. supervalent doping, nanosizing, and subjection to pressure. These were carried out through the exploration of various computational approaches: cluster expansion, ab-initio simulations, and molecular dynamics. The cluster expansion approach was employed to assist in generating new stable structures for the supervalent doping with Ta and W on the Zr site. The Ta-doped structures' electronic and mechanical properties were studied and demonstrated the presence of a band gap of 4.6 eV. alternatively, as an initial approach to understanding the thermodynamic properties of LLZO, the bulk structure was subjected to small pressure during molecular dynamics simulations. Systematic induction of pressure yielded a transition of the tetragonal phase to the cubic phase at 2 GPa pressure. The lattice parameters for the cubic and tetragonal phases, acquired in the study were within 0.38 % agreement with the literature. Furthermore, the XRD graphs confirmed varying phases under different pressure conditions. The temperature phase diagram for 0 GPa structure agreed well with the literature trends and interestingly, the 2 GPa structure retained the cubic phase at various temperatures and was confirmed in the XRDs and temperature phase diagram. The final approach was systematic temperature variation on the bulk and nanostructured LLZO under various temperature conditions in the range 300 − 1500K to understand the LLZO high temperature behaviour and monitor the temperature-induced diffusion. The calculations revealed two distinct patterns of Li-ion transport on the diffusion coefficient plots. The trends in conductive ion diffusions demonstrated that nanostructured materials yielded higher diffusion coefficients than those of the bulk structure. These findings have laid a basis and will contribute towards the evaluation of ionic conductivity and structural stability retention aided by computational simulations.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / **235**

Electronic Stability and Surface Study of Tin Dioxide

Author: khomotso Maenetja[1]

Co-authors: Brian Ramogayana [2]; Phuti Ngoepe

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In lithium-air batteries, metal oxides are frequently regarded as excellent catalysts that help produce stable discharge products and deliver better electrochemical performance. The metal-air battery is a type of electrochemical cell or battery that generates electricity by oxidizing a metal, such as Li, K, Na, or Mg, at the anode and reducing oxygen at the cathode. In this study, we use the density functional theory calculation to investigate the bulk properties and surfaces stability of tin dioxide. Tin dioxide was found to be a stable semiconductor with a band gap of 0.63 eV. The phonon dispersion curves indicate that the structure is vibrationally stable since it shows no soft mode along the brillouin zone direction. The elastic constants show that our structure is mechanically stable since the C' is positive and obey the mechanical stability criteria for a tetragonal crystal. Furthermore, we modelled the low Miller index surfaces which are (110), (101), (111), (001) and (100) from the fully optimised bulk structure using METADISE code. From the modelled surfaces, (110) had the lowest surface energy which is in agreement with the reported literature. The addition of two oxygen atoms revealed the most stable adsorption energy is the bridging configuration was the most favourable. This study

will lead to understanding if tin dioxide will catalyse the oxygen reduction reaction in metal air batteries

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Nuclear, Particle and Radiation Physics / **236**

Development of (p,p'γ) detection capabilities at iThemba LABS through the study of low-lying E1 strength in 58Ni

Author: Refilwe Molaeng[1]

Co-authors: Lindsay Donaldson [2]; Luna Pellegri [3]; Iyabo Usman [4]; Armand Bahini [4]; Wiggert Brümmer [5]; Harshna Jivan [4]; Pete Jones [2]; Sandile Jongile [5]; Kevin Li [5]; Retief Neveling [2]; F. Smit [2]; G. Steyn [2]

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This study aims to test and develop the (p,p'γ) detection capabilities of the K600 magnetic spectrometer when positioned at zero degrees and coupled to the Ball of Germanium and Lanthanum bromide detectors (BaGeL) at iThemba LABS. This is done hrough an investigation into the low-lying dipole strength of 58Ni with a proton beam of Ep = 80 MeV. The use of proton inelastic scattering at forward angles favours the electric dipole excitation and thus gives access to the full strength of the E1 resonance. Detecting these protons in coincidence with the subsequent γ decay improves the selectivity to low spin transfer, allows for the separation of nearby excitations and the assignment of multipolarities. Moreover, the high energy-resolution γ detectors used in decay studies allow for an improvement of the standard energy resolutions obtainable with magnetic spectrometers. The results of this study will be compared to previous experiments to elucidate the advantages of coincidence measurements at iThemba LABS. Important decay paths as well as transition levels will be presented.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics for Development, Education and Outreach / **237**

First year mainstream physics students' conceptions about Kinematics position and displacement concepts

Author: Mark Herbert[1]

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Most first year mainstream physics students of the Department of Physics and Astronomy at the University of the Western Cape generally have difficulty solving problems about Kinematics position and displacement concepts. After the COVID -19 the problems seem to have gotten worse. This paper aims to tell the student's conception of the position and displacement in physics learning. The students' conceptions were derived from test results. The tests and findings will be presented and discussed in this paper.

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics for Development, Education and Outreach / **238**

Improving novice Physical Sciences teachers learning and understanding of basic dynamics by multiple representation in physics

Author: Mark Herbert[1]

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Corresponding Author: dr.ms.herbert@gmail.com

The Department of Physics and Astronomy at the University of the Western Cape partnered with Western Cape Education Department (WCED) in their Teacher Mentorship Programme. The role of the department in the programme is to provide short Continuous Education (CE) courses on different physics topics in the Physical Sciences CAPs curriculum identified by WCED. This paper reports on the Dynamics CE course which aims to improve novice Physical Sciences teachers' learning and understanding of basic dynamics by multiple representation in physics. The impact of the CE course on teachers' learning and understanding was derived from Pre-and Post-test results. In his paper the WCED Mentorship Programme and Dynamics CE course will be described and findings will be presented and discussed.

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 2 / **239**

Novel thermally reduce graphene oxide microsupercapacitor fabricated via mask-free axi-draw direct writing

Author: Vusani Muswa Maphiri[1]

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We demonstrate a simple method to fabricate all-solid-state thermally reduced Graphene Oxide (trGO) microsupercapacitors (μ-SCs) prepared using the atmospheric pressure chemical vapour deposition (AP-CVD) and a mask-free axidraw sketching apparatus. This is a quick, easily operational, cheap, safe, photoresist free, readily scalable method and requires no hazards reducing chemical. The XRD, FTIR and EDS suggest that increasing thermal reducing temperature increases the carbon content within the μ-SC active material. The electrochemical performance of the μ-SCs showed cyclic voltammetry (CV) potential window of 0 - 0.8V at various scan rates (5 – 1000 mVs-1) with a rectangular shape, depicting characteristics of electric double layer capacitor (EDLC) behaviour. The comb-style number of digits per unit area giving the highest capacitance was determined to be 14. The trGO-500 exhibits volumetric energy and power of 13.71 mW h cm-3 and 2677.31 W cm-3, respectively. The electrochemical impedance spectroscopy (EIS) showed the decrease in the equivalent series resistance (ESR) as a function of reducing temperature allotted to reduction of the resistive functional groups present in the sample. Bode plot showed a phase angel of -85 ° for the trGO-500 μ-SC device. The electrochemical performance of the μ-SC devices can be tailed by varying the reducing temperature, number of digits per unity area, and connection configuration (parallel or series).

Apply to be considered for a student ; award (Yes / No)?:

NO

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Consent on use of personal information: Abstract Submission:

Poster Session 2 / 240

Adsorption of H2S on La-ZnO Surface Using DFT+U Method

Author: kharavho shandukani[1]

Co-authors: Ratshilumela Steve Dima [2]; Modjadji Rebecca Letsoalo [3]; Tshifhiwa Steven Ranwaha [3]; Nnditshedzeni Eric Maluta [3]; Rapela Maphanga [4]

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Gas sensing is the detection of toxic gases in the environment/atmosphere for air quality and safety control. It iss based on the principle of transforming the gas adsorption effects on the surface of the active material into a detectable signal in terms of its changed electrical, optical, thermal, mechanical, magnetic (magnetization and spin), and piezoelectric properties. In this work, DFT+U method was used to investigate the properties of H2S adsorbed on to La doped ZnO (101) surface. The calculations are based on the adsorption of H2S on pure and doped with La-ZnO surface to see how doping affects the adsorption process in gas sensing. The calculated lattice parameters are consistent with the experimental results. Doping with La increase the absorption energy.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

Hons

Poster Session 1 / 241

Investigating the effect of sodium partial substitution on nanostructured Li2MnO3 cathodes during the simulated charge process

Authors: Tshidi Mogashoa[1]; Raesibe Sylvia Ledwaba[2]; Phuti Ngoepe[2]

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The exploration of new electrode materials exhibiting improved electrochemical performance and low cost for high-density lithium-ion batteries (LIBs) applicable in electric vehicles is one of today's most challenging issues in material research. Li2MnO3, as a prospective high-capacity (459 mAh.g-1) cathode, suffers from capacity degradation and voltage decay during the cycling process. Incorporating sodium ions in the lithium sites can mitigate voltage decay by limiting transition metal migration, impeding oxygen loss, and improving lithium diffusion of Li-rich layered host materials. In this work, the structural stability of the spherical Li2MnO3, generated through the simulated amorphisation and recrystallisation (A+R) technique was improved by introducing a certain amount of sodium into its lattice structure. The molecular dynamics (MD) calculations were carried out at temperatures between 1600-1800 K, employing the DL –POLY code. Characterisation of the x-ray diffraction (XRD) patterns revealed peak broadening along with the shifting of peaks at 2Θ˜38 to the right due to the enlarged lithium layers occupied by sodium ions to facilitate lithium diffusion. Moreover, the undesired phase transformation from layered to spinel was observed at a later stage of charge for the sodium-doped systems, suggesting that the presence of sodium stabilizes the structure and minimizes the migration of manganese into lithium layers. These findings shed insights on the role of sodium substitution on the nanostructured Li2MnO3 cathodes and will help guide the enhancement of high-capacity energy storage.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 1 / 242

Improve physical properties of rare earth metal doped strontium sulphide for optoelectronic purpose

Author: Samuel Shaka[1]

Co-authors: Mercy Frank [2]; Ikhioya Imosobomeh [3]; Enoh Ogherohwo [4]

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[2] *International Institute of Tourism and Hospitality, Yenagoa, Bayelsa State, Nigeria*

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The electrochemical deposition was used to synthesize SrS-doped zirconium materials at varying dopant concentrations of 0.01 to 0.03 mol. The surface micrograph of the zirconium doped films is well structured on the surface of the FTO used for the synthesis without any crack or lattice strain. The spectrum is polycrystalline with a cubic structure and a prominent peak at (111) orientation for SrS film. At the introduction of the zirconium dopant 0.01 mol, the peak intensity increases with a prominent peak at (211) which indicate acceptance of zirconium dopant in the precursor and as the dopant concentration rises the peak intensity decreases which depicts that a higher concentration of zirconium reduces the peak intensity of the films.The Williamson-Hall plot's slope increases as the dopant concentration increases. The materials exhibit a thickness increase of 121.32 to 126.13 nm and a decrease in film resistivity from 1.12 x 109 to 1.32 x 109 ohm.m, which further led to an increase in conductivity from 7.57 x 108 to 8.26 x 108 S/m.The bandgap energy of SrS is 1.50 eV while SrS-doped zirconium is 1.35 eV − 2.52 eV.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics for Development, Education and Outreach / **243**

Re-Positioning the Department of Physics and Astronomy at UWC for Natural and Physical Sciences teachers training and development

Author: Mark Herbert[1]

Co-authors: Bako Audu [2]; Ronald Engelbrecht

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[2] *UWC*

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A review of undergraduate physics education in public higher education institutions undertaken by the South African Institute of Physics (SAIP) in partnership with the Council of Higher Education (CHE) has identified the major challenge of the under-preparedness of university students entering undergraduate physics programmes as a teacher development problem. As a result, student throughput and retention at universities remain a very large concern for higher education in South Africa. The Department of Physics and Astronomy, in response to the SAIP call to Physics Departments in South Africa to get involved with the training and development of teachers to address the under-preparedness of learners in our schools, established the Department Teachers' Training and Development Programme. The programme is an initiative of the Department in collaboration with the UWC Faculty of Education, Metro Education Districts in the Western Cape Education Department (WCED), Cape Peninsula University of Technology and the University's partner in the USA, the University of Missouri-Columbia. The programme aims to increase the critical mass of learners that are needed in the Science, Technology, Engineering and Mathematics (STEM) sector in South Africa by improving the physics content knowledge and pedagogical skills of Natural and Physical Sciences teachers and thereby increasing learners' interest, participation and success in the Natural Sciences and Physical Sciences in our schools. In this presentation, the programme will be described as well as its successes and challenges.

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 2 / **245**

First-Principles Study of sodium De-intercalation From Tri-Chalcogenide NaNbSe2

Author: Sana Sana[1]

Co-authors: Ratshilumela Steve Dima [2]; Tshifhiwa Steven Ranwaha [1]; Nnditshedzeni Eric Maluta [1]; Rapela Maphanga [3]

[1] *University of Venda*

[2] *University of venda*

[3] *CSIR*

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The importance of energy generation and storage cannot be overstated, given rising energy demands and the depletion of fossil fuels. Because of their low cost, abundance of elements, strong reversibility, and moderate energy density, sodium-ion batteries have piqued interest as a possible alternative for large-scale electrochemical energy storage. To provide critical fundamental insights into electrode materials and to ease the development of materials for sodium-ion batteries, computational techniques have been widely used in connection with experimental investigations. In this work we investigated the electrochemical performance of the transition metal chalcogenide NaNbSe2 as a material for sodium-ion batteries using systematic first-principles calculations based on density functional theory employing the generalized gradient approximation. The 2 × 1 × 1 super-cell is used for our research on NaNbSe2. Because of the slight distortion of octahedron, the simulation lattice was set to the P1 space group. The comparison of lattice parameters from the relaxation structure and previously experimental results was done and the calculated results were consistent with the experimental results.

Apply to be considered for a student ; award (Yes / No)?:

YES

Level for award;(Hons, MSc, PhD, N/A)?:

Hons

Poster Session 2 / **246**

Control and monitor the operation of PVWPS using the OVH SCADA-based system

Author: Livhuwani Masevhe[1]

Co-authors: Eric Musandiwa Mulovhedzi [2]; Eric Nnditshedzeni Maluta [1]

[1] *University of Venda*

[2] *Spider Black*

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The water pumping system in the agricultural sector is one of the major users of photovoltaic solar energy particularly in off-grid locations. For an optimal functioning of the system to be achieved, a real-life monitoring tool can provide the farmer or operator to be in-charge and be able to control the system remotely. In the current study, a monitoring the influence of meteorological parameters on the PV power generation, soil temperature and water-loss due to evaporation and absorption. A proposed open-source Supervisory Control and Data Acquisition (SCADA), the OVH SCADA 4.0 application for a photovoltaic water pumping system is discussed in this paper. The activities of logging of parameters such as environmental parameters like temperature; humidity; light intensity; soil moisture, hydro parameters like water level; water flow rate into and out of the tank, and electrical or solar parameters such as solar panel voltage; battery voltage capacity; and load current were discussed comprehensively. The purpose of the monitoring system is to provide a useful tool for the operation and management of the PVWPS using the RTU-1600AP where data was pushed using GSM second generation communication to an open source OVH SCADA 4.0 cloud system upon which data was able to be visualized and interpreted.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Applied Physics / **247**

Density functional theory study of Ti-doped NaMnO2, a cathode material for sodium-ion battery

Author: Tshifhiwa Steven Ranwaha[1]

Co-authors: Ratshilumela Steve Dima [2]; Nnditshedzeni Eric Maluta [1]; Rapela Maphanga [3]

[1] *University of Venda*

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Due to the accessibility of Na resources and comparable performance to lithium-ion batteries, rechargeable sodium-ion batteries are popular for large-scale electric energy storage and smart grids. attributed by its benefits, NaMnO2 is a promising cathode material for Na-ion rechargeable batteries. However, Na has a lower ionization potential than Li, resulting in lower operating voltages and energy densities than LIBs. Na+ ions are heavier and larger than Li+ ions, resulting in slow diffusion within a solid electrode during SIB cycling and often larger electrode volume expansion. In this study, we used the cluster expansion formalism to investigate the Ti-doped NaMnO2 phase stabilities, predicting the stable multi-component crystal structures and ranks metastable structures by enthalpy of formation while maintaining the predictive power and accuracy of first principle density functional theory method. The binary diagram produced 30 new structures of stable phases from which only five structures are stable. The stable structures obtained from the binary diagram have different space groups, different lattice parameters, the same Wyckoff positions and a different energy of formations. The optimised structures have a cross validation score of 1.1 meV which is an indication of a good cluster expansion because it has CVS lesser than 5 meV per active position.

Apply to be considered for a student ; award (Yes / No)?:

YES

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Theoretical and Computational Physics / 248

Short path length corrections to pQCD phenomenological energy loss models in a QGP

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Co-author: William Horowitz [1]

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The standard model of particle physics has been used to successfully describe observables from particle collisions at high energies in colliders such as the LHC and RHIC. In the last twenty years evidence for the formation of a substance known as Quark Gluon Plasma (QGP), has been found in heavy-ion collisions (collisions of atoms with a large number of nucleons). This substance probes the most interesting and complicated sector of the standard model - Quantum Chromodynamics (QCD). The QGP is a nearly ideal fluid which existed around 20μs after the Big Bang, and is made up of the freely interacting fundamental degrees of freedom in QCD - quarks and gluons. Phenomenological perturbative QCD (pQCD) models describing QGP formation involve many moving parts: a model for the non-perturbative, fluctuating, initial conditions of the collision; a hydrodynamics simulation of the fluid; a perturbative QCD model for both radiative and elastic energy loss; and a model for the hadronization of quarks and gluons into final state hadrons. With all of these inputs and theoretical uncertainties, the success of predictions of various phenomenological models is astounding. An open and fascinating question in this field, is how big does a collision system have to be before QGP is formed? In particular it is not known whether there is QGP formation in systems such as proton + heavy-ion ($p + A$) or even high-multiplicity proton+proton ($p + p$) collisions. The current theoretical tools are often ill-equipped to deal with small systems; and the validity of thermal field theory, and hydrodynamics in these small systems is not known. In this talk I will introduce some phenomenological models which have been used to successfully describe observables related to the formation of QGP in heavy ion collisions; as well as talk about our original work being done to allow existing pQCD energy loss models (WHDG, DGLV) to be used for predictions related to QGP formation in smaller systems ($p + p$ and $p + A$) collisions.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics of Condensed Matter and Materials Track 1 / 250

Computational study of electronic and optical properties of graphene/brooki composite

Author: lutendo phuthu[1]

Co-author: Nnditshedzeni Eric Maluta [1]

[1] *University of Venda*

Corresponding Author: phutulutendo@gmail.com

Recently, carbonaceous nanomaterials such as carbon nanotubes and two-dimensional graphene have attracted the attention of the scientific community in probe to improve energy conversion and storage technologies. The graphene sheet is more preferred due to its large specific area, flexible structure, high transparency, excellent mobility of charge carriers and is expected to be able to slow the charge recombination. Graphene/Transition metal oxides nanocomposite study has become much of a wide interest recently with metal oxides like TiO2 and ZnO. These metal oxides are used as thin films in photovoltaic technology to harness energy. The final composite embodies both the transport properties of the former and the semiconducting properties of the latter species. This work describes an analysis of the electronic and optical properties of graphene/TiO2 studied using the Density Functional Theory (DFT) in application to dye-sensitized solar cells (DSSCs).

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics of Condensed Matter and Materials Track 1 / 251

Synthesis and Characterization of Caesium Lead Tri-Iodide by Sequential Physical Vapour Deposition for Solar Cells

Author: Sizwe Sibiya[1]

Co-author: Mmantsae Diale [2]

[1] *Abstract*

[2] *University of Pretoria*

Corresponding Author: drbheki636@gmail.com

In this study, we report on the synthesis and characterization of titanium dioxide thin film prepared via the spray pyrolysis technique. X-ray diffractograms confirmed a tetragonal crystal structure with an average crystallite size of 24.44 nm and a micro-strain of 9.75x10-4. Field-emission scanning electron micrographs show pin-hole-free and densely packed grains with an average size ranging from 25 to 29 nm. UV-Vis spectra revealed an absorption onset 300 nm for the film. The estimated film bandgap was 3.9 eV.
The sequential physical vapour deposition technique was used to grow quality thick films of metal halide perovskites in a safe, scalable, and reproducible manner. Growth of high-quality poly-crystalline yellow phase caesium lead tri-iodide (CsPbI3) was refined by varying the CsI thickness from 200 nm to 500 nm. Crystallographic parameters and phase transitions from as-deposited orthorhombic γ-CsPbI3 to tetragonal β-CsPbI3 on annealing at 100 ℃, were determined using X-ray diffraction patterns. Computed lattice constants were a= 4.88 Å, b= 9.96 Å, and c= 16.52 Å, with an average crystallite size increasing from 169.46 nm to 243 nm, and the micro-strains decreased with an increase of CsI thickness. The field-emission scanning electron micrographs showed a uniform surface covered with polycrystalline grains. The Average grain size increased from 168 to 235 nm as the caesium iodide (CsI) thickness increased, resulting in large pin-hole-free and tightly packed grains. A 2.24 to 2.38 eV increase in the bandgap was observed when CsI thickness was increased. Herein, we demonstrated optimized structural, morphological, and optical properties of CsPbI3 for use in solar cells, grown via sequential physical vapour deposition technique for stable and completely inorganic perovskites.
Finally, the electrical properties of fabricated FTO/TiO2/CsPbI3/Au devices were characterized using the current-density (I-V) measurement technique. Although the CsI thickness varied, it had no effect on the cell's performance because the devices showed consistent power conversion efficiency of about 4%. Moreover, the open circuit voltage shows a decreasing trend when CsI thickness decreases.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / **252**

Computational studies of optoelectronic properties of CH3NH3PbI3 as a photolayer in perovskite solar cell

Authors: Elkana Rugut[1]; Nnditshedzeni Eric Maluta[2]; Rapela Maphanga[3]; Edwin Mapasha[4]; Joseph Kirui[5]

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[2] *University of Venda*

[3] *Council for Scientific and Industrial Research*

[4] *university of pretoria*

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Structural, electronic, mechanical and optical properties of pseudo-cubic CH3NH3PbI3 were investigated using density functional theory. The predicted values of the stated properties agreed reasonably well with the existing theoretical and experimental data. Optical studies were undertaken so as to probe the photo-physical properties of the material in order to gauge its suitability as the absorber layer in solar cell based on many body pertubation theory by solving the Bethe-Salpeter equations. Optical descriptors such as the reflectivity, refractive index, absorption coefficient and energy loss as functions of photon energy were extracted from the numerical data of the real and imaginary part of the dielectric function as per the Krammer-Kronig relations.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Nuclear, Particle and Radiation Physics / **253**

Investigating the excess of two same-sign and three lepton final states via four top quark production

Authors: Thuso Mathaha[1]; Bruce Mellado[2]; Mukesh Kumar[2]

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Despite the discovery of the Higgs boson at the Large Hadron Collider (LHC) confirming the SM's predictions, additional scalar bosons may exist as long as their mixing with the SM Higgs is minimal.

The 2HDM model with a singlet scalar extension has been shown to accurately explain multi-lepton anomalies at the LHC, where the heavy scalar has a mass of $m_H \approx 270$\,GeV, and the singlet scalar has a mass of $m_S \approx 150$\,GeV. The excess production of two same-sign leptons and three isolated leptons with b-jets has been observed by both the ATLAS and CMS experiments. This study focuses on the CP-odd scalar of the 2HDM+S model, the heavy pseudoscalar (A), with a mass between 400-600\,GeV. The heavy pseudoscalar primarily decays into $t\bar{t}$, ZH resulting in four top quarks and four lepton final states. This research investigates the production of two same-sign and three leptons from four top quark final states produced by $t\bar{t}A$ ($A \rightarrow t\bar{t}, ZH$) and compares the production mechanisms of four top quarks in the SM and beyond the SM.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Theoretical and Computational Physics / 254

Computer simulated study of the structural and electronic properties of β-MnO2 nanoclusters as cathode materials in rechargeable lithium-ion batteries

Authors: Phala Masoga[1]; Hasani Chauke[1]; Phuti Ngoepe[1]

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Computer simulated study of the structural and electronic properties of β-MnO2 nanoclusters as cathode materials in rechargeable lithium-ion batteries

1,2 P.W. Masoga, 2P.E. Ngoepe and 2H.R. Chauke

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Significant attention has recently been focused on transition metal-oxides due to their allotropic polymorphs having distinct structural and electronic properties. Pyrolusite (β-MnO2), the most stable polymorph of MnO2, is one of the most promising cathode materials necessary for the creation of improved rechargeable battery systems such as lithium-ion batteries.
In this study, MnO2 nanoclusters were produced using an evolutionary algorithm and first principle methods. Interatomic potentials were used in conjunction with the Buckingham potential and the 12-6 Lennard-Jones potential to generate subsets of stable nanoclusters. A combination of global search techniques and density functional theory (DFT) methodologies were used to refine the energy ordering of the generated nanoclusters and determine their global minima.
The selected interatomic potentials predicted the β-MnO2 bulk structure to within 0.43 % of experimental data. The Ni-doped n3-01 nanocluster on the cation position with the higher coordination was the most stable, most compact and had the highest operational voltage profile of 3.038 V showing nickel to be the preferred dopant in this study. The generated x-ray diffraction patterns for the stable nanoclusters revealed the most dominant and stable peaks with their respective intensities' indicative of the stable rutile phase. Furthermore, the effect of temperature changes on nanocluster stability was studied. The nanoclusters showed a preference toward circular compact bonding patterns at higher temperatures. There are improvements in the stability and electrical conductivity in the nanoclusters as compared to bulk β-MnO2. The DOS revealed that the nanoclusters are metallic at the Fermi level with small band-gap energies. Due to its advantageous electrical conducting qualities and the fact that co-doped nanoclusters had the smallest band-gap energies, Co-doping also

demonstrated some potential. The charge density differences of the Ni-doped n3-01 nanocluster displayed a high prevalence of covalent bonding as opposed to ionic bonding observed with Fe- and Co-doping further showing nickel to be the preferred dopant.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / **255**

Analysis of calculated and measured entrance skin dose of common radiographic procedures.

Author: Ejeh Ernest[1]

Co-authors: Ochai-Ejeh Faith [2]; Ugwe Kenneth [2]; Ohagwu Christopher [3]; Audu Innocent [4]

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This work reports the result of the comparison between calculated entrance skin dose (ESD) and measured entrance skin dose using thermo-luminescent dosimeter (TLD) in a teaching hospital in North Central, Nigeria. The exposure parameters and anthropometric characteristics of twenty (20) adult patients exposed to X-ray radiation at the Benue State University Teaching Hospital, Makurdi, North Central for chest X-ray examination (10 patients) and abdomen X-ray examination (10 patients) were recorded. The measured ESD data were compared to Edmonds model, Faulkner model, Chougule model, Davies model, and Kepler model. The entrance skin doses (ESD) of two common radiographic examinations determined by the use of Lithium Fluoride Thermo-luminescent dosimeter were found to be generally low when compared to the ESD obtained by mathematical model. The measured ESD from this work was lower than the DRLs values.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 1 / **256**

Ion beam modification of PANi-PMMA blends for hole transport layer applications in perovskite solar cells

Authors: Eulanda Eulanda[1]; Msimanga Mandla [2]; Masenya Mamogo[2]

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Polymer solar cells (PSCs) are a promising alternative for low-cost renewable energy due to their flexibility, simplicity in synthesis, and large-area fabrication. Methyl ammonium lead halide-based hybrid perovskite solar cells (PSCs) have been extensively studied in recent years because of their high efficiency and low processing costs. Long-term stability, however, remains a challenge as constituent layer materials are susceptible to UV radiation damage and environmental degradation. Polyaniline (PANI), a chemically and thermally stable conducting polymer, shows potential to serve both as a protective barrier and an efficient hole transport layer. Blending PANI with a structurally stable polymer like polymethyl methacrylate (PMMA) can address the issue of brittleness and cracking in pure PANI films during drying after spin coating, though at the expense of the electrical conductivity. To enhance the conductivity of the PANI-PMMA blends while maintaining their mechanical stability, doping is crucial. Metal ion implantation offers precise control over dopant dose and distribution, in contrast to conventional chemical doping methods. This paper reports on the structural, optical, and electrochemical characterization of pristine and 30 MeV Au7+ ion-irradiated PANI-PMMA blend films with varying PANI weight concentrations. The topography of the films was investigated with atomic force microscopy (AFM), ultraviolet-visible (UV-Vis) spectroscopy provides insights into the optical properties, while electrochemical measurements assess the activity and stability of the blends. The results highlight the potential of ion beam modified PANI-PMMA blends as hole transport layer materials in perovskite solar cells, contributing to their optimization for renewable energy applications.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics for Development, Education and Outreach / **257**

Repositioning the Department of Physics and Astronomy at the University of the Western Cape for Learners Programme

Author: Bako Nyikun AUDU[1]

Co-authors: Mark Herbert [2]; Ronald Engelbrecht [3]

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[2] *UWC*

[3] *Metro South Education District*

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The Department of Physics and Astronomy at the University of the Western Cape (UWC) has been involved in collaborating with stakeholders in the engagement of High school learners for better achievement at various stages of basic education. This is done to enhance and improve learners' retention in the education system, access to next-level movement within the system, success at standard examinations, and throughput for the general health of the education system and its beneficiary systems. The Department of Physics and Astronomy in collaboration with the Metro South Education District has taken this quest further by engaging with High Schools in the Cape Flats to design intervention at the community level with high schools to ensure significant growth and improvement in learners' achievement, learners' interest and learners' participation in Mathematics and Physical sciences. Within the scope of the department's outreach is the focus on the need to produce students who can follow careers in the Sciences, Technology, Engineering, and Mathematics (STEM) stream and to develop individuals to attain their full potential in life. The programmes

undertaken by the Department of Physics and Astronomy improved the pass rate for grades 8 and 9 mathematics for 2018 was over 10%, grade 11 for 2019, and grade 12 for 2022 were inconclusive due to data protection issues respectively. The plan for the 2023 engagement is on the verge of being concluded and will form part of the presentation. The study will present the goal of the intervention, identify factors that encourage learners' retention in such programmes, challenges, and successes.

Keywords: Physical Science, Mathematics, Intervention, Retention.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / 258

The Use of a Burn-in Station for Stress-Testing of the LVPS back-end electronics for the Tile Calorimeter

Author: Tristan Jade Wilkinson[1]

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Abstract. The Tile Calorimeter (TileCal) is a hadronic sampling calorimeter which forms a part of the ATLAS detector, one of the major experiments at the Large Hadron Collider (LHC). As part of the scheduled Phase-II upgrade of the LHC, and subsequently TileCal, the backend electronics are undergoing an upgrade to their Low Voltage Power Supply (LVPS) systems; electronics have a high mortality rate in the first few months of deployment, which necessitates the development of a method for testing electronics to ensure the minimisation of these early-stage fatalities. A burn-in station is a sophisticated system which artificially ages the electronics, while monitoring the input and output loads that each individual circuit board is experiencing - which can ultimately be used to ensure that the produced electronic components can function with minimal chance for failure.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics of Condensed Matter and Materials Track 1 / 259

Investigating hydrogen induced Ti3Al embrittlement in Ti-6Al-4V using TEM

Authors: Velile Vilane[1]; Robert Knutsen[2]; Johan Westraadt[1]

[1] *Nelson Mandela University*

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Temporary hydrogen alloying (THA) can refine coarse-grained as-cast Ti-6Al-4V microstructures and improve tensile strength. However, it can also reduce the tensile ductility to severe embrittlement because of hydrogen promoted titanium aluminide (Ti3Al) precipitation.[1] The effect of oxygen concentration above a 0.33 wt.% threshold on Ti3Al promotion is known.[2] The effect of residual hydrogen concentration above a 150-ppm threshold on Ti-6Al-4V embrittlement is also known.[3] Less Known is the effect of hydrogen on the promotion of Ti3Al precipitation, and the effect of precipitated Ti3Al on tensile ductility. This study investigates hydrogen promoted Ti3Al precipitation, and its effects on the tensile ductility of hydrogenated-dehydrogenated (HDH) Ti-6Al-4V.

A hydrogenation-dehydrogenation (HDH) treatment was used to refine a coarse-grained Ti-6Al-4V microstructure with the intention of optimizing its tensile strength and ductility. Microstructure evolution was characterized using X-ray diffraction (XRD), electron backscatter diffraction (EBSD), energy dispersive spectroscopy (EDS) and transmission electron microscopy (TEM). Oxygen and hydrogen concentrations were quantified using inert gas fusion (IGF).

The results indicate that HDH treatment does not refine the coarse network of prior beta grains, but it alters the coarse Widmanstätten microstructure by nucleating submicron beta grains within the individual lamellae. The HDH modified microstructure had higher ultimate tensile strength (UTS) in the order of 100 MPa. The dehydrogenation temperature affected tensile ductility; the lowest dehydrogenation temperature (675 °C) had the highest ductility loss in the order of 75%. Increasing the dehydrogenation temperature recovered ductility until full ductility was recovered at 750°C. The ductility loss was not caused by residual hydrogen or oxygen but was caused by the embrittling effect of hydrogen induced Ti3Al which remains in the microstructure even after hydrogen removal, and only completely dissolves at a Ti3Al solvus temperature of 750 °C. The results demonstrate that HDH treatment alters the initial coarse-grained Ti-6Al-4V microstructure to extents that significantly improve strength, but it also promotes Ti3Al precipitation and its concomitant embrittlement. To improve ductility, the dehydrogenation treatment should be controlled to optimize Ti3Al dissolution.

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Apply to be considered for a student ; award (Yes / No)?:

n/a

Level for award;(Hons, MSc, PhD, N/A)?:

n/a

Poster Session 2 / 260

The role of Physics in sustainable development

Authors: Aluwani Guga[1]; Sunday Ogundipe[2]; Yondela Mdlatu[2]

Co-authors: Shandukani Muronga [2]; Vhuhwavho Phophi [3]; Asenathi Qushu [1]; Azwinndini Muronga [2]

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During the United Nations General Assembly in September 2015, the 17 Sustainable Development Goals (SDGs) were approved, and to achieve these goals, we must work as a team. All of these SDGs require a basic knowledge of the sciences in order to be achieved. In order to ensure a world that is balanced, sustainable, and inclusive, the International Year of Basic Sciences for Sustainable Development 2022 will be an important moment for mobilization to convince economic and political leaders, as well as every citizen, that Basic Sciences are vital to securing a sustainable, balanced world. There is a fundamental need for a fundamental understanding of both natural phenomena and those generated by human imagination and organization in order to implement Agenda 2030. Having a fundamental understanding of nature will enable all interested parties to perform actions more effectively for the benefit of all. Herein we report on how physics contributes to sustainable development goals. Aiming to improve the well-being of both people and the planet while ensuring sustainable use of natural resources.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Astrophysics & Space Science / 261

On some nuances of time-dependent galactic cosmic ray proton modulation

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The study of galactic cosmic ray (GCR) antiparticles can potentially lead to new insights into fundamental physics, in particular in the search for indirect evidence of dark matter annihilation. Identifying the signature(s) of such processes, however, is complicated by the heliospheric modulation of these particles. Modulation becomes less significant at higher energies, and therefore it would be of interest to ascertain at which energy such effects become negligible. Although previous studies have reported on this, to date no attention has been given to the influence of solar cycle-dependent effects. The present study aims to do so, using our 3D, fully time-dependent ab initio GCR modulation model, that can reasonably fit both proton and antiproton observations over multiple solar cycle. Furthermore, the influence of time-dependent GCR modulation on potential signals of dark matter annihilation will be investigated.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 2 / 262

Towards a Century of Physics in South Africa: Achievements and Advances

Authors: Aluwani Guga[1]; Yondela Mdlatu[2]; Shandukani Muronga [3]; Sunday Ogundipe[1]; Vhuhwavho Phophi [3]; Asenathi Qushu[3]; Azwinndini Muronga [2]

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South African physics dates back to 1751 when Nicholas Louis de Lacaille made significant astronomical observations of the southern sky at the Cape of Good Hope. Also, at Cape Town's Royal Observatory, John Herschel began investigating double stars, clusters, and nebulae between 1834 and 1838. In the second half of the 19th century, geomagnetic and surveying work was introduced, and several universities and colleges were established. Following the establishment of the mining industry in the early 20th century, physics research in several universities in the country gained popularity.
In 1923, South Africa became a founding member country of the IUPAP, bringing physics to international prominence. South Africa has witnessed tremendous growth in physics, including international collaborations, research institutes, infrastructures, facilities, scientific innovations, discoveries, and inventions. In this study, we present an overview of the significant achievements and innovations made by South African physicists between 1920 and the current century as a result of the study of physics.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

Hons

Physics of Condensed Matter and Materials Track 2 / 263

Investigation of structural, electronic, elastic and dynamical properties of Li2Mn0.5Ru0.5O3 cathode material for Li-ion batteries: A first-principles study

Author: Mamonamane Mphahlele[1]

Co-authors: Cliffton Masedi [2]; Kemeridge Malatji [3]; Phuti Ngoepe [2]; Raesibe Sylvia Ledwaba [2]

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Li₂MnO₃ has been considered as one of the promising cathode materials for lithium-ion batteries due to its high theoretical capacity, nontoxicity, and natural abundance of Mn. However, it has not been commercialized due to poor structural stability and low conductivity during cycling. To ameliorate the electrochemical performance of Li₂MnO₃, we propose doping with Ru, which can stabilize the structure and improve its electronic conductivity.
In this study, the cluster expansion technique was used to generate new phases of Li₂Mn_{1-x}Ru_xO₃ (0≤x≤1) with varying concentrations and symmetries. The binary phase diagram predicted Li₂Mn_{0.5}Ru_{0.5}O₃

as the most stable phase with the lowest negative heats of formation, suggesting thermodynamic stability. In addition, the elastic constants for Li₂Mn_{0.5}Ru_{0.5}O₃ satisfied the required stability criterion for triclinic structures, indicating mechanical stability. The phonon dispersion curves showed no negative vibrations along high symmetry directions of the Brillouin zone, suggesting that the doped phase is dynamically stable. Moreover, the density of states shows a decrease in the band gap of Ru-doped Li₂MnO₃ from 1.506 eV to 0.417 eV, which leads to higher electrical conductivity of the material. Finally, based on these results Li₂Mn_{0.5}Ru_{0.5}O₃ can be proposed as potential cathode materials for use in lithium-ion batteries, which may lead to improved cycling performance.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Theoretical and Computational Physics / **264**

Equation of state and the Casimir effect in non-Abelian gauge theory on the lattice

Author: Blessed Arthur Ngwenya[1]

Co-authors: Alexander Rothkopf [2]; William Horowitz [1]

[1] *University of Cape Town*

[2] *University of Stavanger*

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We present a study of the equation of state in finite-temperature non-Abelian gauge theory for isotropic and anisotropic lattices, where the temperature T is varied by changing the temporal lattice size N_t at fixed lattice scale a. We compute the trace anomaly and the corresponding pressure/energy density and show the lattice spacing, as well as the volume dependence, with the corresponding the jackknife statistical error analysis. We also present results of the Casimir potential and the Casimir mass in $SU(2)$ at zero-temperature in $(2+1)$ spacetime dimensions, studied through the introduction of two parallel chmomoelectric wires separated by a distance R on the lattice plaquettes. We show that the attractive Casimir interaction varies exponentially with the distance between the wires and is damped at large separation between the wires.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Astrophysics & Space Science / **265**

Multi-messenger analysis of Ultrafaint dwarf galaxies as observational targets for Dark Matter indirect detection

Author: Raees Noorbhai[1]

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The dwarf spheroidal galaxies orbiting the Milky Way galaxy, particularly the Dark Matter-dominated Ultrafaints, possess excellent discovery potential as observational targets for DM indirect detection. We assess hypothetical, leptophilic WIMPs in the 1 TeV–2 TeV range, with four dwarf galaxies chosen as potential observational targets. These are the Classical dwarf galaxies Sculptor and Sextans, along with the Ultrafaints Reticulum II and Segue 1. For gamma ray observations, we consider the CTA and LHAASO telescopes. For neutrino observations, we consider the KM3NeT infrastructure, while for radio observations we consider the MeerKAT infrastructure. Utilising conservative estimates of the telescope sensitivities, we project non-detection constraints imposed by observations of the dwarf galaxies within the field-of-view of each telescope, calculating upper bounds upon the velocity-averaged annihilation cross-section of the WIMP. Our multi-messenger analysis thereafter compares the projected non-detection bounds imposed by observations of the Ultrafaint dwarf galaxies to those imposed by observations of the Classicals, for the different telescopes and their corresponding astrophysical messengers. These projected constraints are taken in comparison to those imposed by prior DM indirect searches in Reticulum II, the Large Magellanic Cloud and the MW Halo and Centre. Also taken into consideration are the direct detection constraints, the collider search constraints, the CMB constraints and the DM relic density limit. Thus, the analysis allows us to determine the optimum combination of telescope infrastructure, astrophysical messenger and target dwarf galaxy for the purposes of imposing the strongest non-detection constraints upon the WIMP parameters.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Nuclear, Particle and Radiation Physics / **266**

Increasing the location rate of Positron Emission Particle Tracking (PEPT) measurements at PEPT Cape Town

Authors: Rayhaan Perin[1]; Jonathan Shock[1]; Kathryn Cole[1]; Stephen Peterson[1]

[1] *University of Cape Town*

Corresponding Author: rayhaanperin1@gmail.com

Positron Emission Particle Tracking (PEPT) is a non-invasive particle tracking technique used to study particle and fluid transport in a range of applications, including medicine and chemical engineering. PEPT produces time-series 3D location data, however the output rate of locations is limited by the timing resolution of the equipment used. At PEPT Cape Town at the University of Cape Town, the in-house positron emission tomography (PET) scanner is a Siemens "EXACT3D" HR++ which records coincidence data to the nearest "timestamp" of 1 ms. Therefore a maximum location rate of 1 kHz is used for PEPT measurements to avoid introducing additional uncertainty to the time of each location measurement. For some applications, this is insufficient to track the highest frequency components of the motion of the tracer particle. To investigate the uncertainty in the time of each location, we developed a simulation of the HR++ and moving tracer particles in GEANT4 (GEometry ANd Tracking 4) Application for Tomographic Emission (GATE). Our results suggest a value for the uncertainty in the time measurement of each location and ways in which the precision of the time of each coincidence event can be increased. The implementation of PEPT measurements with higher locations rates will improve the accuracy of measurements of the average velocity of

the tracer particle, which is especially important for tracking the fluctuating velocity components characteristic of turbulent flows.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Physics of Condensed Matter and Materials Track 1 / **267**

Synergistic effects of Au on the gas sensing properties of Yb-doped Co3O4-In2O3 nanostructures

Authors: Rethabile Makole[1]; Hendrik Swart[2]; David Motaung[2]

[1] *University of the Free State*

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Noble metals such as Ag, Au, and Pt have been reported to improve gas sensor sensitivity by inducing electronic and chemical sensitization of the sensor layer. This is one of the methods used to enhance the gas response of metal oxide semiconductors for the detection of volatile organic compounds (VOCs). Monitoring of emitted VOCs in industrial and residential spaces serves as a precautionary measure for possible exposure to emissions exceeding the recommended limits. Herein, we report on the detection of BTEX compounds, which are aromatic VOCs using Au-loaded ytterbium-doped Co3O4-In2O3 nanostructures at a working temperature of 100 ˚C.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Theoretical and Computational Physics / **268**

Modeling and tomographic visualization of the dying Schrodinger cat and its implication for the biomechanical dynamics of cardiovascular diseases

Author: Godfrey Akpojotor[1]

Co-authors: Moses Imah [2]; Sharon Egboro [3]; Akpan Ettong [2]; Famous Akpojotor [4]; Hamzah Yusuf [1]; Paul Akpowaide [1]

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The dying Schrodinger cat is modeled in this study as a simple harmonic oscillator using the usual various steps of modeling. The formulated constitutive equation of the dying cat developed is a second order differential equation with physical constant coefficients which includes three crucial components: the damping constant, b, which represents the quantity of poison the cat is exposed to, the spring constant, k, which represents blood flowing in the cat's heart and the cat's mass, m. The constitutive equation is numerically solved and simulated for varying amount of poison, blood flowing in the heart and cat mass. Both the numerical results and the tomographic visualization depicted the following three states with time and energy: underdose state in normal sinusoidal motion and energy, critical dosage state in anomalous sinusoidal motion and highly reduced energy, and overdose state in quenched sinusoidal motion and energy. This study motivated our modeling strategy of assuming that the physiological state of the presence of the cardiovascular disease (CVA) in the infected person (IP) can be physically described as the superposition of the characteristic wave of the disease on the characteristic wave of the healthy person (HP). The resultant superposed wave is the constitutive carrier wave equation which can be solved to provide the biomechanical dynamics of the IPs and are depicted in an electrocardiogram (ECG). The prospect of using this approach for the prognosis of the physiological state of cardiovascular diseases is then discussed.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Theoretical and Computational Physics / 269

Theoretical & Computational Biophysics

Authors: Fundile Nyaweni[1]; Ntokozo God-knowledge Cebekhulu[2]; Asakundwi Praisethelord Dzhivhuho[2]; Dineo Patience Motjope[2]; Funanani Raphulu[2]; Dephney Mathebula[2]; Rendani Netshikweta[2]; Mercy Moila [2]; Aluwani Guga[2]; Azwinndini Muronga[2]

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The project explores the interlinked of biophysics, biomathematics and biostatistics; and further examine the application of deterministic models in biological systems using COVID-19 as a case study. The deterministic model, which utilizes the classical SEIR epidemic modeling framework, is used to determine the transmission dynamics of the COVID-19 epidemic. The objective of the project is to develop a deterministic model of COVID-19 and fit it to South Africa's COVID-19 data in order to gain insight into infectious disease dynamics by translating mathematical results back to biology and by using numerical algorithms to study the physical principles behind infectious diseases. The fitted model was found to fit the recovered group data well, but not the infected group. Hence, the importance of fitting the data for COVID-19 modeling, allows researchers and policymakers to use the models for predictions and inform decision-making. However, this model needs to be improved in order to fit the data.

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Applied Physics / 270

Density functional theory study of Porphyrin dye molecule adsorbed on TiO2 (010) Anatase surface.

Author: Ronel Ronella Randela[1]

Co-authors: Tshifhiwa Steven Ranwaha [1]; Lutendo Mathomu [1]; Rapela Maphanga [2]; Nnditshedzeni Eric Maluta [1]

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Dye-sensitized solar cells (DSSCs) have attracted considerable attention in recent years as they offer the possibility of low-cost conversion of photovoltaic energy. DSSCs use the dye molecules adsorbed on the TiO2 semiconductor in nanoarchitecture with the role of absorbing photons from the sun. In this study, Density functional theory (DFT) has been used to study the geometric, electronic, and optical properties of Pheophytin dye and its adsorption behaviour on (010) TiO2 anatase surface. The generalized gradient approximation (GGA) was used in the scheme of Perdew-Burke Ernzerhof to describe the exchange-correlation function as implemented in the CASTEP package in the material studio of BIOVIA. The results obtained show that Pheophytin dye molecules can improve the efficiency of DSSCs as they show an absorption shift to the near-infrared region, which increases the absorption range on the visible solar spectrum.

Key words: DSSC, DFT, Porphyrin Dye

Apply to be considered for a student ; award (Yes / No)?:

YES

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Applied Physics / 271

Long-term kimberlite activation for Radiological Assessment for the Min-PET technique.

Authors: Thendo Emmanuel Nemakhavhani[1]; Simon Conell[None]; Martin Cook [None]; Gideon Bentum[2]; Jaco Houman[None]

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This study presents the activated and background sample activity results of different mined rocks from the Letseng diamond mine and the radiological impact due diligence simulated activation stage of the Mineral-Positron Emission Tomography (Min-PET) technique performed at Aarhus University. The activated and background-specific activities were validated by irradiating the kimberlite rocks with a 40 MeV photon beam and will not lead to any long-term radiological concerns. The

Min-PET technique is the process by which a diamond is detected within the activated kimberlite rocks by the Min-PET detectors. The 100 MeV Aarhus microtron injector has been degraded to 40 MeV using a 2.3 mm stainless steel, 5 mm copper plate. The beam was a further incident on a 3 mm thick tungsten layer to produce bremsstrahlung photons for a long-term kimberlite activated to transmute the ^{12}C (γ, n)^{11}C to release back-to-back 511 keV gamma photons to be detected by two planar Min-PET detectors. The rocks were placed 800 mm away from the beam exit and were irradiated for 10 minutes and cooled for another 10 minutes. The longer cooling period leads to the activated isotopes such as oxygen that have a half-life of fewer than 10 minutes to decay off to the background level. After cooling time, the rocks were sent to High Purity Germanium detectors (HPGe) for data/spectra of the long half-life isotope acquisition. This step was also done for non-irradiated rock samples to identify the naturally occurring background isotopes. The energy spectra from the HPGe detectors data were used to identify the energy of each peak in the spectra and the online nuclear database was used to identify the isotope of each energy peak. The specific activities of the natural background and activated radionuclides were calculated by fitting a Gauss in each energy peak on the energy spectra. The natural background-specific activities resulting from an unirradiated sample were found to be 4.95 mBq/g for ^{40}K, and 2.85 mBq/g for 511 keV. The specific activity results for activated isotopes were studied in three stages of data acquisition, firstly a short-term activation (between 10 minutes and 15 hours after activation) where it was found to be 1004 mBq/g for 511 keV, 5.32 mBq/g for ^{40}K, and 400 mBq/g for ^{24}Na, secondly for medium-term activation (between 15 hours to 1 day after activation) were found to be 3.0 mBq/g for 511 keV, 4.2 mBq/g for ^{40}K, and 0 mBq/g for ^{24}Na respectively. The activated sample's specific activities decrease with time, but, still within the acceptable range recommended by IAEA for long-term activation. The natural background-specific activities and specific activities from activated rocks remain constant and are comparable in all different samples. These results proved and validated the Min-PET technique to be safer for any long-term radiological concerns.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Nuclear, Particle and Radiation Physics / **272**

Photoabsorbtion Cross-Section of Mg 24.

Author: Jacob Bekker[1]

Co-authors: Luna Pellegri [2]; Lindsay Donaldson [3]; Retief Neveling [3]

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Accurate nuclear data is a key factor in determining the suitability and reliability of many theoretical nuclear models and large scale calculations. This is especially true for cases where the systematic calculations are challenging such as light and deformed nuclei.The photoabsorption cross section and the relative branching ratios for these nuclei are of particular interests to investigate their nuclear structure and also for their usage in modeling of astrophysics scenarios as the propagation of ultra high energy cosmic rays (UHECRs). The presented project investigates the total photoabsorption cross section via excitation of the giant dipole resonance of 24Mg, one of the keystone nuclei in these propagation simulations. The giant dipole resonance was probed using 200 MeV protons via the virtual photon production method. This was done at the iThemba LABS facility using the Separated Sector Cyclotron and the K600 Spectrometer in the zero degree configuration mode. The high resolution focal plane detection suite combined with the Eikonal model for virtual photon production proved to be an effective combination for extracting

the electromagnetic response of light nuclei as is shown in the 24Mg case. The obtained photoabsorption spectrum is presented alongside the total photoabsorption cross section obtained from real gamma measurements as well as a comparison to data from RCNP, Japan using the GRAND Raiden spectrometer.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Photonics / **273**

Photonic crystal-based biosensing for TB detection

Author: Charles Maphanga[1]

Co-authors: Saturnin OMBINDA-LEMBOUMBA [2]; Yaseera Ismail [3]; Patience Mthunzi-Kufa [1]

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Corresponding Author: cmaphanga@csir.co.za

Over the last three decades, biosensors based on photonic crystals (PhCs) have been developed and continue to receive significant recognition owing to their distinctive electromagnetic properties and broad applications. Studies that have used refractive index as a parameter to design optical biosensing devices based on PhCs have resulted in optical devices that are sensitive with quick response time for small variations in samples. In this study, a 1-dimensional (I-D) PhC biosensor chip was developed for the diagnosis of TB. A pathogen-specific mycolic acid (MA) TB biomarker was studied based on the detection of refractive index changes on functionalised PhC biosensing surface. The MA biomarker was used as the biorecognition element to capture anti-mycobacterium tuberculosis antibodies, and a custom-built optical biosensing setup was used for optical biosensing to monitor biomolecular interactions between the antigen and antibody. Functionalised and successfully characterised gold nanoparticles (AuNPs) were introduced on the biosensing surface to enhance the detection signal. The biosensing surface was further characterised using atomic force microscopy (AFM), scanning electron microscopy (SEM), and energy-dispersive X-ray (EDX) spectroscopy. Analysis of biomolecular binding events on the biosensing surface was achieved using the optical biosensing setup by measuring transmitted light through the biosensor chip, and successfully distinguishing differences between the experiment and control samples. From our findings, it was realised that mycolic acid antigen can be used as a biomarker for active TB, and can be successfully immobilised on a biosensing surface to capture anti-mycobacterium tuberculosis antibodies. It was evident that PhC-based optical biosensing technique was successful in detecting small refractive index changes on the biosensing surface for the diagnosis of TB. These results pave the way toward the development of a PhC-based point-of-care (POC) diagnostic device for TB.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Applied Physics / 274

Nuclear Orientation Thermometry using the UCT Dilution Refrigerator

Author: Yanga Ntolosi[1]

Co-authors: Steve Peterson [2]; Mark Blumenthal [3]

[1] *NMISA*

[2] *Department of Physics, University of Cape Town*

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The development of a Nuclear Orientation (NO) thermometer system for use at the University of Cape Town is essential to address the significant challenge in the accurate measurements at ultra-low temperatures (down to 8mK). A $^{60}CoCo(hcp)$ gamma-ray thermometry source was irradiated using the NECSA SAFARI-1 research reactor for 6 minutes and a preliminary activity value of 1.3 MBq was achieved. The activity of this source has been validated using an absolute gamma-ray coincidence technique and verified using a well-type ionizing chamber. Preliminary temperature measurements were taken by placing the ^{60}Co source within the University of Cape Town Department of Physics dilution refrigerator using a vertical sample holder and measuring the anisotropy of the radiation at a 90 ^{0} angle using a Sodium Iodide (NaI) scintillation detector. These results were promising, but inconclusive, prompting a second set of measurements. Modifications were made to the experimental set up by re-designing the sample holder to hold the source horizontally and take measurements at 0 ^{0} angle along the c-axis. A Lanthanum Bromide $(LaBr_3)$ scintillation detector was also used to measure the radiation at temperatures ranging from 10 mK to 100 mK. These experimental improvements provided more accurate and conclusive results.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / 275

Quantum state inference from coarse-grained descriptions: analysis and an application to quantum thermodynamics

Author: Paola Concha Obando[1]

Co-authors: Raul O. Vallejos [2]; Pedro Silva Correia ; Fernando de Melo [2]; Alexandre B Tacla ; Nina Machado ONeill [2]

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Whether considering our everyday perception of the surrounding environment or a sophisticated experimental setup, a characterization of a physical system is given in terms of measurement results of its observable properties. Thus, given that this characterization is not unique, it is necessary to consider which features are being observed as well as how they are being observed. In this context, the aim of state inference is to assign to the system a description that abides by the know data. In this work, we discuss two ways of assigning a description to a quantum system assuming that

we have a coarse-grained access to its properties. Specifically, we compare the maximum entropy principle method, with the Bayesian-inspired average assignment map method [Correia et al., Phys. Rev. A 103, 052210 (2021)]. Despite the fact that the assigned descriptions by both methods respect the measured constraints, and that they share the same conceptual foundations, the descriptions differ in scenarios that go beyond the traditional open quantum system-environment structure. The average assignment map is thus shown to be a more sensible choice for the ever more prevalent scenario of complex quantum systems. We discuss the physics behind such a difference, and further exploit it in a quantum thermodynamics process.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / **276**

Microstructure and strain dependence on growth time of hydrothermally synthesized nanocrystalline porous sodalite

Authors: KYALO Ngesu KITEME[1]; G L Kabongo[1]; M S Dhlamini[1]

[1] *UNISA*

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In the present report we demonstrate the synthesis of sodalite NaAlSiO2 nanocrystals via hydrothermal process. Moreover, the synthesized nanostructured materials were obtained at different growth time which systematically revealed its effective dependence along with the crystallinity and surface morphology. In addition, the as-synthesized nanomaterials were characterized using various analytical techniques such as X-ray Diffraction, SEM microscopy and EDS spectroscopy. Finally, microsctructure dependence on growth time was systematically demonstrated for crystalline NaAlSiO2 nanoparticles porous morphology and crystallite size ranging from 14 to 38 nm.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

Msc

Physics of Condensed Matter and Materials Track 1 / **277**

Using the sf-model to describe spintronic devices

Author: Volkmar Nolting[1]

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Crystals containing rare earth atoms are interesting candidates for spintronic devices due to the fact that magnetism and the electric current are caused by different electron groups. The exactly solvable zero bandwidth limit of the sf-model is used to calculate the conduction electron spin polarization P(T,n), the chemical potential $\mu(T, n)$ and the 4f-magnetization m(T,n). The results confirm the existence of spin dependent electron transport properties in these materials. As an application to 4f-antiferromagnetism the alloy series $CeNi_{1-x}Co_xGe_2$ is investigated. It is shown that the susceptibility X(T) displays a peak at the Neel temperature T_N thereby indicating a transition into the paramagnetic phase. A numerical evaluation yields results in qualitative agreement with those of other authors.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / 279

STUDY OF THE IMMOBOLISATION OF PALLADIUM BY SILICON AND ZIRCONIUM IN GRAPHITE.

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Current high temperature gas reactor designs use TRISO-coated particles as fuel. The TRISO-coated particle consists of a fuel kernel and coating layers of porous pyrolitic carbon (PyC), inner high-density PyC, silicon carbide (SiC) and outer high-density PyC. The SiC layer serves as the main barrier to fission product release1. However it has been reported that the radioactive fission product Ag110m can escape from intact TRISO particles2. It was also found that the fission product palladium (Pd) significantly enhances the migration of silver along grain boundaries in SiC3,4.

This paper investigates the feasibility of using Pd traps such as Si and ZrC in the inner PyC layer of TRISO particles to capture the Pd and prevents it from migrating to the SiC layer by forming immobile silicide compounds in the case of Si. It is proposed that without Pd in the SiC, the migration rate of Ag in SiC will be significantly reduced.

Graphite discs (used to simulate PyC) were implanted with 137,5 keV Si and 190 keV Zr ions to doses of 8,27 x1015 Si ions cm-2 and 5x1015 Zr ion cm-2. Pieces of implanted graphite discs, with a layer of Pd powder on the implanted surface, were subsequently annealed for 20 min. at temperatures of 600 and 900 ℃. TEM samples were cut using a focused Ion Beam (FIB) and analysed using a JEOL 2100 TEM.

Fig. 1 (a) is a cross-sectional HAADF STEM micrograph of Si implanted graphite annealed in contact with Pd powder at 600 ℃ for 20 min. The bright particles are the Pd on the Si implanted graphite as indicated in the figure. Fig. 1 (b) is a HAADF STEM micrograph showing the location of the EDS line scan across a Pd particle and into the Si implanted graphite. The corresponding EDS line scans for Pd, C and Si are shown in (c) together with the location of the implanted graphite surface. The similarity of the Pd and Si line scans indicate that at 600 ℃, the Si rapidly diffused out of the graphite and into the Pd particles. The same result was obtained after annealing at 900 ℃ for 20 min. which is indicative of the high chemical reactivity of Pd and Si to form a silicide3. The current study revealed that the palladium silicide formed will most likely be immobile in graphite (and PyC) at temperatures up to 900 ℃.

The EDS results of the Zr implanted graphite annealed in contact with Pd at 600 and 900 ℃ indicated that Zr did migrate into Pd but the reaction was less pronounced than that found for Si. The incor-

poration of Si into the inner PyC layer of a TRISO particle during manufacturing would be easier and more effective as Pd trap than ZrC.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc Physics

Astrophysics & Space Science / **281**

Dark matter searches with MeerKAT

Authors: Geoff Beck[1]; Michael Sarkis[2]; Natasha Lavis[2]

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The nature of dark matter remains a major unresolved mystery in modern cosmology. In this work we explore the use of the MeerKAT Galaxy Cluster Legacy Survey in placing limits on the allowed annihilation cross-section for a variety of possible WIMP models. In so doing we demonstrate that MeerKAT is competitive with best available results in the literature, excluding WIMPs annihilating into b-quarks with masses below 800 GeV as viable cosmological dark matter. This unexpectedly makes galaxy clusters, with their large baryonic backgrounds, competitive with dwarf galaxy results.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Photonics / **282**

Mid infrared gas absorption spectroscopy using a photonic chip-based supercontinuum

Author: Proficiency Munsaka[None]

Co-authors: Peter Baricholo ; Gurthwin Bosman. W ; Rohwer Erich. G [1]

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We report the simulation of ultrafast pulse evolution along a silicon germanium waveguide. Pulse evolution of 205 fs duration and 2.35 kW peak power at 4.15 μm propagating through a 5 cm long silicon germanium on silicon substrate waveguide was simulated by solving the generalised nonlinear Schrödinger equation using the fourth order Runge-Kutta in the interaction picture method. Coherent supercontinuum covering more than one octave from 2.61 μm to 8.15 μm (relating to a

bandwidth of 5.54 μm) at -30 dB was achieved. This simulated mid infrared spectra was used in the simulation of gas absorption spectroscopy for carbon dioxide and methane gases. Absorbance spectra of these greenhouse gases were calculated from the resolution of the Beer-Lambert equation. The computed absorbance spectra agree well with the absorbance spectra found on the high-resolution transmission (HITRAN) spectral database.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics of Condensed Matter and Materials Track 1 / 283

Synthesis and modification of Boron Nitride nanotubes using ion implantation

Author: Lehlohonolo Lisema[1]

Co-authors: Trevor Derry [1]; Morgan Madhuku [2]; Rudolph Erasmus [3]; Daniel Wamwangi [4]; Adam Shnier [5]; David Billing [3]

[1] *School of Physics, University of Witwatersrand, Johannesburg 2050, South Africa*

[2] *iThemba LABS*

[3] *University of the Witwatersrand*

[4] *School of Physics, Materials Physics Research Institute, University of the Witwatersrand*

[5] *University of Witwatersrand*

Corresponding Author: 1701761@students.wits.ac.za

In this work, Chemical Vapour Deposition (CVD) has been used to synthesize boron nitride (BN) nanostructures, particularly nanotubes, and defects selectively introduced into the synthesized BN nanostructures through ion implantation. Scanning electron microscopy (SEM) images show clear evidence of BN nanostructures and BN nanotubes (BNNTs), with the latter appearing as long, thin structures with diameters ranging from ⊠30-90 nm. Raman analysis show an E_2g mode of vibration assigned to hexagonal BN (hBN) at 1366 cmˆ-1 after ion implantation, with increased intensity. Grazing incidence X-ray diffraction (GIXRD) spectra revealed a prominent peak, a (004) hBN characteristic peak, present in the 54°-56° angle region, which was used to determine the average lattice parameters (a⊠2.23 and c⊠3.64 Å), crystallite size ⊠5.60nm and density (⊠1.75g/cm3) of BN nanostructures. The most notable observation in this study was a significant rise in the size of the crystallite domains in the nanostructures synthesized at 1100 and 1200 ℃ after ion implantation with boron ions at fluence 5x10ˆ14 ions/cmˆ2.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Applied Physics / 284

Artificial neural network-based photodiode radiometer for instantaneous global solar irradiance measurements

Author: Olebogeng Tlhapane[None]

Co-authors: Raphael Mukaro ; Ashmore Mawire

Corresponding Author: 21443394@nwu.ac.za

A low-cost, BPW21 Si-photodiode-driven solar radiometer was designed and used for long-term measurement of global horizontal solar irradiance. This was necessitated by the fact that the Kipp & Zonen CMP11 pyranometer available in the department and used as the secondary standard pyranometer, is expensive for most of our running renewable energy projects. A data acquisition system (DAS) was used to simultaneously measure the radiometer and the CMP11 voltages, as functions of time of day. Artificial neural networks (ANNs) were then used to calibrate the radiometer voltages against the CMP11 calculated irradiances. A data set spanning four months was collected and used to create, train, test, and validate the networks. During training, radiometer voltages and time of day were inputs to the ANNs, while CMP11 irradiances were the targets. Data for selected days not used in the training were then used to test and validate the ANNs. The photodiode sensor used has an acute spectral response compared to the CMP11. Despite this setback, ANNs were successfully used to match radiometer and CMP11 irradiances. This novel approach returns instantaneous global horizontal irradiances for the entire day. Root-mean-square error (RMSE), mean absolute error (MAE) and mean absolute percentage error (MAPE) was used to assess the performance of the radiometer. The design matched the CMP11 with RMSE values ranging from 10 W/m2 to about 22 W/m2, with a standard deviation of about 1 W/m2. The average MAPE was 3.5%, while the average MAE was 6 W/m2.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 1 / 285

Heat-up approach of inorganic aliphatic Co(II) complexes to form CoS quantum dots for quantum dots sensitized solar cells

Author: MOJEED ADEDOYIN AGORO[1]

Co-author: Edson Meyer [2]

[1] *UNIVERSITY OF FORT HARE*

[2] *University of Fort Hare*

Corresponding Author: magoro@ufh.ac.za

Nanoscience research has shown a drastic increase in metal nanoparticles in various fields compared to their corresponding Group V and VI counterparts. This can be attributed to their unique properties, easy to harness, high surface atoms, which promote better active sites with unique electronic properties between the metallic and molecular states. Specifically, metal sulfides have a variety of sulfur-containing ligands that are easily tunable and can have their decomposition kinetics and secondary decomposition products optimized by controlled modification using precursors like dithiocarbamates (DTCs). Extensive studies are yet to be conducted on cobalt sulfide (CoS) to explore the strong coexistence of reducible cobalt with oxidizable sulfur ions as compared to other metal sulfide semiconducting materials. In the present study, we demonstrated the intriguing structural, optical, and morphological properties of CoS quantum dots for dye-sensitized solar cells (DSCs). The photosensitizers were characterized by TGA, FTIR, SEM, EDS, TEM, UV-Vis, and PL. The X-ray diffraction pattern for the prepared CoS@a, CoS@b, and CoS@c nanoparticles matched well with the hexagonal

and cubic phases of CoS and CoS2. The energy band gap of 1.7–2.3 eV for the three samples implies that these materials are better candidates for QDSSCs and energy storage device applications. This is further supported by SEM analysis for CoS@a and CoS@c with nano-rod micrographs, which are known as catalysts for enhancing electrical conductivity. The thermolysis of the three molecular precursors using a single-source approach below the boiling point of the coordinating solvent produces CoS without impurity. We believe that the fascinating macro/nanostructure obtained in this study can be explored in different applications, such as QDSSCs.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Theoretical and Computational Physics / 287

First principles characterization of nitrogen dopant- vacancy complexes in graphane

Author: Hezekia Mapingire[1]

Co-author: Refilwe Edwin Mapasha [2]

[1] *University of Pretoria*

[2] *Pretoria University*

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We compute first principles calculations to characterize four types of point defects in the 2-dimensional material graphane. The point defects we consider in this contribution are nitrogen dopant-vacancy complexes and their various charge states. We compute the formation energies, binding energies, U-parameters and other electronic properties of these impurity-vacancy complexes in graphane monolayer with the objectives of utilising this group of point defects for quantum computing. Analysis of DOS plots and defect level diagrams shows that the complex formed by a nitrogen dopant substituting a carbon atom adjacent to a hydrogen vacancy exhibit interesting properties that may make this point defect complex a possible qubit candidate. Charge neutrality pins the fermi level at a value close to 2eV deep between the VBM and the CBM making this complex a deep centre defect.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Theoretical and Computational Physics / 289

Exploring the connections between quantum search algorithms and ghost imaging

Authors: Paola Concha Obando[1]; N. Gounden[None]; Andrew Forbes[2]; Issac Nape[3]

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[2] *U. Witwatersrand*

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Corresponding Author: paola.conchaobando@wits.ac.za

Quantum ghost imaging is a non-invasive imaging technique that involves non-local photon pairs. One photon from an entangled pair interacts with the object while the other non-integrating photon is directed to a spatially resolved imaging detector. In this context, the analysis of the spatial correlations of these two spatially separated photons enables the reconstruction of the image of an object. We show that by looking at quantum ghost imaging from a quantum computation perspective, a remarkable link between the ghost imaging and quantum search algorithms can be found. In this talk, I will present the main results showing the close relation between the quantum operators that connects both process, as well as the discuss how this link allows us to explore quantum computation tasks from the quantum optics perspective.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 2 / **290**

Sinc related Basis functions with predetermined nodes

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The sinc function is defined by

$\text{sinc(x)} = \sin \pi x \frac{}{nx.}$

with $\text{sinc(0)} = 1$ and $\text{sinc(i)} = 0$ for $\text{i} \neq 0$.

Defining

$\text{s}_i^{(h)} sinc\frac{(x-i)}{h} gives a set of interpolating functions with nodes \text{ih}. However in some instances it is more desirable to h$

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Astrophysics & Space Science / **291**

Statistical analysis of ground level enhancement (GLE) and Forbush decrease (FD) using neutron monitor data covering solar cycle 23 and 24.

Author: Lehlogonolo Arnold Phasha[1]

Co-authors: Nndanganeni Rendani [1]; Sivakumar Venkataraman [2]; Mpho Tshisaphungo [1]

[1] *SANSA*

[2] *University of KwaZulu-Natal*

Corresponding Author: phasha497@gmail.com

The main aim of this study is to perform statistical analysis of ground level enhancement (GLE) and forbush decrease (FD) associated with solar events, such as coronal mass ejections (CMEs), solar energetic particles (SEPs) and solar flares. The study will also investigate which of the solar events has the greatest influence in terms of GLEs and FD magnitudes. The period of study covers the solar cycle 23 and 24, 1996-2008 and 2009-2019 respectively. Within these two solar cycles, 18 GLE events were observed by the neutron monitors (NM) world-wide. This study will consider the data from the four NM stations in the southern hemisphere namely; Hermanus, Potchefstroom, Tsumeb and SANAE. These solar events will be investigated independently, and the preliminary results will be presented and discussed in this paper.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / 292

Exploring the spectroscopy of the low and medium spin states in ˆ{148}Sm Nucleus.

Authors: Mfundo Zuma[1]; Ntshangase Sifiso[2]

[1] *none*

[2] *Supervisor*

Corresponding Author: mf04ndo@gmail.com

The ^{148}Sm nucleus has Z=60 protons and N=86 neutrons. The neutron number represents only 4 neutrons above the N=82 shell gap. In the N=86 isotones, the competition between collective and single-particle modes of excitation results in a formation of different kinds of excited level structures. The observed structures are interpreted as due to octupole vibrational states coupling with the single particle excitation resulting in alternating-parity bands linked by electric dipole 1 transitions. The dynamical fluctuations associated with the coupling to low-lying quadrupole and octupole vibrations(=) are also expected in these isotones. The low-lying quadrupole vibrational states in ^{148}Sm have not been measured, and the spins and parities in some states of this nucleus remains unknown. Thus, this work seeks to search for the low- and medium states in 148Sm, and to also determine the spins and parities of the excited states, which could subsequently allow one to understand the microscopic nature of the structures reported in the previous studies. In the present study, the excited states in ^{148}Sm are populated following the ^{148}Nd (^{4}He, 4n) ^{148}Sm reaction at a beam energy of 47.0 MeV. The iThemba LABS AFRODITE array is used for detection of γ- radiation from the reaction, the established level scheme will be expanded based on the $\gamma - \gamma$ coincidence measurements. The AFRODITE array consisted of 9 High-Purity Germanium (HPGe) detectors, 5

positioned at 90° and 4 at 135°. Spin and parity assignments are made based on angular distribution and linear polarization measurements

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Nuclear, Particle and Radiation Physics / **293**

In situ radionuclide analysis at a rehabilitated contamination site using a mobile gamma-ray detection unit equipped with a LaBr3:Ce detector

Author: Ferdie van Niekerk[None]

Co-authors: Pete Jones ; Stephan Woodborne

Corresponding Author: fvniekerk@tlabs.ac.za

Carbonatite-peralkaline complexes represent the major type of host rock for phosphate in South Africa. It is well known that this rock also contains small amounts of naturally occurring uranium and its decay products. The spillage of polluted process water during December 2013 at the Bosveld Phosphates mine in Phalaborwa, South Africa, lead to the run-off of this water into the adjacent Selati River that runs through the Kruger National Park (KNP). This caused concern for possible radiation pollution in the river and surrounding ecosystems. It is known that the site has since been rehabilitated. A mobile radiation detection unit equipped with a LaBr3:Ce detector was used to perform in situ radiation measurements at two sites in the KNP, one unaffected by the process water spillage and the other being the contaminated site itself. Real-time activity data, synchronised with GPS coordination, was collected at both sites. Analysis of the spectral data and radiation mapping indicated successful rehabilitation as no elevated radiation levels were observed at the previously contamination site compared to the unaffected site. Results obtained during the experimental measurements will be presented and discussed, and conclusions drawn during the presentation.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics of Condensed Matter and Materials Track 1 / **295**

The development of Ti-Pt-V shape memory alloys using both computational modelling and experimental techniques

Author: Rosinah Modiba[1]

Co-authors: Pfarelo Daswa [1]; Charles Siyasiya [2]; Silethelwe Chikosha

[1] *CSIR*

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There is currently a high demand for the development and commercialisation of TiPt based shape memory alloys (SMAs). The development of these SMAs involves both computational modelling and experimental techniques. The integration of both techniques provide a detailed interpretation of the results that cannot be achievable using only the experimental approach. Therefore, this study uses first principles computational modelling and experimental techniques in the development of Ti-Pt-V alloys. Titanium (Ti)-based alloys are considered to be the most attractive metallic materials for aerospace and automobile applications. In this regard, the TiPt alloys are the most promising SMAs for high temperature application due to their transformation temperature of above 1000 0C. However, the binary alloys have been found to be mechanically unstable and exhibit very low shape memory effect, which is attributed to low critical stress for slip deformation compared to the stress required for martensitic transformation. Therefore, the addition of alloying elements has been suggested as one of the ways to improve the mechanical properties of TiPt alloys. In this study, the addition of 6.25 and 12.5 at.% vanadium (V) to replace either Ti or Pt was used. It was observed that both approaches were in good agreement wherein the replacement of Ti with V increased the martensitic transformation temperature of the TiPt alloys. However, the reverse was observed with the replacement of Pt with V.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Applied Physics / 296

Shaping a kaleidoscope of colours

Author: Leerin Michaela Perumal[1]

Co-author: Andrew Forbes [2]

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[2] *U. Witwatersrand*

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Since the late 1990s, laser beam shaping has experienced a surge in activity. With the use of modern digital tools, one has the power to tailor light in its many degrees of freedom (polarisation, amplitude and phase) to create so-called ‘structured light’. In recent years we have seen structured light used in various fields such as optical communication, information processing, detection, imaging and even industrial manufacturing. With advancements in the various fields, the demand for broadband structured light has increased as it offers an additional degree of freedom to manipulate. In the past decade modulation of multiple wavelengths has been achieved with devices such as spatial light modulators (SLMs). However, these devices are polarisation dependent, costly and have slow response rates- making it unsuitable for many commercial uses. Digital micromirror devices (DMDs) on the other hand are polarisation and wavelength independent, compact, cheaper and have an extremely fast response rate. In this work we show how broadband beam shaping can be achieved by adding a single lens after the DMD and observing the beam in the image plane. The experimental results correlate well with the theory, thus validating the approach. In this way, we offer a simple cost-efficient and versatile tool for the modulation of broadband or in theory any desired wavelength of light.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / **297**

Overview of Ion Beam Analysis (IBA) actitivities at iThemba LABS-NRF

Authors: Mlungisi Nkosi[1]; Christopher Mtshali[2]; Ntombizonke Kheswa[2]; Nametso Mongwaketsi[2]; Zakhele Khumalo[3]; Lebogang Kotsedi[2]; Mamogo Masenya Mamogo[4]; Mandla Msimanga[5]; Phillip Sechogela[2]; Morgan Madhuku[2]

[1] *Head of Tandetron Laboratory*

[2] *iThemba LABS*

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[5] *Tshwane University of Technology*

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iThemba LABS is a facility that houses various research accelerators, including the latest 3 MV TandetronTM accelerator, which was installed in 2017 to replace the 51-year-old 6 MV CN Van de Graaff accelerator. High Voltage Engineering Europa B.V. (HVE) was responsible for installing and commissioning the new accelerator in the Tandetron Laboratory. The accelerator has the ability to accelerate charged particles to MeV energies from three ion sources, including a Cs sputter source for heavy ions and two multi-cusp ion sources for helium ions and protons. The primary purpose of the accelerator is to facilitate research in ion beam analysis (IBA) and low-energy astrophysics.

The 3 MV TandetronTM accelerator is linked to the experimental section through 90-degree analyzing and switching magnets that direct the charged particle beam into the experimental chambers. Currently, two active beam lines are designated for solid-state physics techniques like Rutherford Backscattering Spectrometry (RBS) and Elastic Recoiled Detection Analysis (ERDA), as well as nuclear microprobe-based techniques such as Particle-Induced X-ray Emission (PIXE) and proton beam writing. Another beam line is under commissioning for astrophysics-related research projects.

The ion sources available with the accelerator can produce high-intensity beams of 200 eμA and 25 eμA for protons and helium light ions, respectively, and a maximum of 150 μA for heavy ions at the terminal voltage of 3 MV. This makes the accelerator particularly promising for materials research areas such as ion implantation, radiation hardness testing, and shielding studies.

The Tandetron laboratory has recently expanded its research areas to include studies associated with laser-matter interaction using femtosecond lasers, diffusion kinetics studies in nuclear waste storage materials and hydrogen storage materials, measurement of fundamental parameters in ion-matter interactions, and surface texturing or patterning using proton beams.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Photonics / **298**

Quantum Algorithms on Classical Optical Vector-Matrix Multipliers

Author: MWEZI KONI[1]

Co-authors: Bezuidenhout Hadrian ; Andrew Forbes [2]; Isaac Nape [3]

[1] *University of the Witwatersrand*

[2] *U. Witwatersrand*

[3] *Structured Light Lab, School of Physics, University of Witwatersrand*

Corresponding Author: 1856324@students.wits.ac.za

Matrix-vector multiplication is a crucial operation in quantum algorithms such as Deutsch-Josza's, Grover's, and phase estimation. Here we present an approach that uses classical light to perform similar operations. We demonstrate this technique by directing light onto pixelated liquid crystal Spatial Light Modulators (SLMs) that encode information on the spatial pattern of light to create a matrix. When the light beam passes to the next SLM, we can perform element-wise matrix multiplication. The intensity of each element is proportional to the product, allowing for efficient computation. We begin by discussing the fundamental principles behind optical vector-matrix multipliers and show that our redefined element-wise matrix multiplication with a cylindrical lens acting as a summing operator is equivalent to the standard equation describing matrix-vector products, and then present our implementation of several well-known quantum algorithms, demonstrating their effectiveness.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

Msc

Photonics / **299**

Is classical entanglement of a vector beam fragile or robust?

Author: MWEZI KONI[1]

Co-authors: Isaac Nape [2]; Andrew Forbes [3]

[1] *University of the Witwatersrand*

[2] *Structured Light Lab, School of Physics, University of Witwatersrand*

[3] *U. Witwatersrand*

Corresponding Author: 1856324@students.wits.ac.za

Vector beams are characterized by their non-separable (entangled) polarisation and spatial degrees of freedom. However, different views persist on the entanglement's robustness against phase-perturbing turbulent media: on one hand the entanglement should be robust, on the other it decays. This work is aimed at reconciling the two contradictions, by experimentally and theoretically studying vector beams, entangled via their orbital angular momentum modes and polarisation degrees of freedom through a turbulent media. Using a quantum mechanical framework, we show that turbulence results in the broadening of the OAM spectra, and by performing the measurement in the original basis we lose information. However, by performing basis-independent measurements, we show that entanglement is invariant against phase perturbations and the state remains non-separable. Thus, showing how you measure determines what you see.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / 300

Search for a Higgs boson decaying to a four lepton plus missing transverse energy final state via four vector bosons

Author: Xola Mapekula[1]

Co-author: Matthew Connell [1]

[1] *University of Johannesburg*

Corresponding Author: chesta101@gmail.com

This analysis presents the search for the Standard Model Higgs that decays to a pair of dark Higgs to an eight-lepton final state via four dark vector bosons.
In this scenario, the SM Z boson can kinetically mix with the $U(1)_D$ gauge boson Z_D while the dark Higgs S and the SM Higgs can exhibit mass mixing. Either of the Higgses can can be formed from gluon-gluon fusion and decay to the other type of Higgs which in turn can decay to a Z_D pair.The overall topology envisioned is $H \rightarrow SS \rightarrow Z_D Z_D Z_D Z_D \rightarrow 8\ell$, which gives an eight lepton final state where ℓ could be ν, e or μ.
The probability of observing different configurations of the final states was calculated. We compared these results to the observed final states from generated samples and found that they agreed. In the case where we observe four detectable leptons(e or μ) and four undetectable leptons (ν), an investigation was then done to see whether the visible leptons pairs from the same S particle (denoted as the 4-4 case) or different S particles (2-2-2-2 case). We then developed a discriminator based on the angular kinematics of each event in order to separate the 4-4 case from the 2-2-2-2 case. The discriminator was found to work for specific values of the parameter phase space, while in the other phase space th data was found to be irreducible.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Applied Physics / 301

Imaging with X-rays and prospect of a cold neutron source at Necsa

Authors: Robert Nshimirimana[1]; Lunga Bam[2]; Jakobus Hoffman[2]; Evens Moraba[2]

[1] *NECSA*

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The South African Nuclear Energy Corporation (Necsa) is in the process of establishing a neutron beam line center (NBLC) that will benefit South African researcher community and industries. The NBLC will grow and expand its capabilities at a proposed new build of a multi-purpose reactor facility which will include a cold neutron source. Imaging instruments with neutron/X-ray/gamma source, will form part of the NBLC to support and fulfil the mandate of Necsa in undertaking and promoting research and development in the field of nuclear energy, radiation sciences, and technology development. Currently, a facility capable of imaging with X-ray is well-established at Necsa, and a thermal neutron imaging facility is under an upgrade at SAFARI-1 research reactor. The imaging center has become a multidisciplinary research facility with utilization in non-destructive testing, cultural heritage, agriculture, energy sector, civil engineering, bio-sciences, metallurgy, and geo-sciences. This talk showcases the capabilities of imaging with X-rays, and the prospect of imaging with a cold neutron source at Necsa.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Photonics / **302**

Pumping up the frequency conversion of structured light

Author: Sachleen Singh[1]

Co-authors: Bereneice Sephton [2]; Imogen Morland [3]; Mitchell A. Cox [4]; Jonathan Leach [5]; Wagner Tavares Buono [2]; Andrew Forbes [6]

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Frequency conversion of light with orbital angular momentum (OAM) such as Laguerre-Gaussian (LG) beams is important for various applications such as free-space optical communications, sensitive infrared light detection, and obtaining OAM lasers. Traditional methods of frequency conversion involve a nonlinear medium and two input beams i.e., a signal LG beam and a pump beam with either flat-top or plane wave or gaussian profiles which suffer from significant loss of pump photons. To overcome this issue, we introduce the concept of pump shaping. By utilizing pump beams with specific shapes, such as amplitude-ring and annular-ring, we experimentally demonstrate a significant improvement in the frequency conversion efficiency and purity of the output mode. Our approach employs Difference Frequency Generation (DFG), a second-order nonlinear process, but can be extended to other processes, such as Sum Frequency Generation (SFG) and Second Harmonic Generation (SHG), offering a highly efficient solution for frequency conversion of structured light.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / 303

Phase characterisation of a deformable mirror through digital Stokes polarimetry

Author: Light Mkhumbuza[None]

Co-authors: Keshaan Singh [1]; Andrew Forbes [2]; Angela Dudley [3]

[1] *University of the Witwatersrand*

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Deformable mirrors have predominantly been used in a wide range of fields such as adaptive optics due to the robustness they possess in terms of aberration correction. In this work we utilise the combination of interferometry and digital Stokes polarimetry to characterize the wavefront emerging from a deformable mirror. We achieve this by interfering two fields of orthogonal polarisation whereby one polarisation acts as the reference beam with a known phase and the other is reflected from the deformable mirror with an unknown phase. These two beams then propagate to a Spatial Light Modulator and subsequently a polarisation grating to separate the orthogonal polarisation components, allowing one to extract all four Stokes parameters needed to determine the intramodal phase.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / 304

The study of the properties of Titanium based alloys for biomedical applications using the First Principle' approach.

Author: Kobe Mabeba[1]

Co-authors: Enoch Sithole [2]; Rosinah Modba [3]

[1] *Student*

[2] *Sefako Makgatho Health Sciences University*

[3] *CSIR*

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ABSTRACT
Titanium (Ti) and its alloys have been widely used as implant materials due to their outstanding mechanical characteristics and biocompatibility. Some of the applications includes orthopedic, and endoderm surgeries etc. However, there is a great concern regarding the difference in the implant material's Young's modulus and that of natural bone. With prolonged use, Ti alloys releases dangerous ions to the human body hence the need to improve the Young's moduli of these alloys. The aim of the study is to investigate the structural and mechanical stability of Ti-Mg-Si alloys using first principle approach. The elastic properties and the Density of States (DOS) of the alloys were determined by the first-principle calculations based on the Density Functional Theory (DFT) using Cambridge Serial Total Energy Package (CASTEP) and the results were compared with the available

experimental results. Cubic Ti-Mg-Si tends show a rise in the density of states peak near the fermi line. In conclusion Mg contribution to the structure Ti-Mg-Si leads to a formation of a metallic bond and increased elasticity which confirms the mechanical and structural stability.

Key words: Properties of Titanium based alloys, Structural and Mechanical stability of Ti-Mg-Si alloys, DFT, First-Principle.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / **305**

The study of Zr and Nb alloyed on the beta-Ti for bio-medical applications: first principle approach.

Author: Thabiso Mathews[1]

Co-authors: Enoch Sithole [1]; Rosinah Modiba [2]

[1] *Sefako Makgatho Health Sciences University*

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Abstract:
Titanium alloys have been used in the bio-medical industry since the 1800s.They are incredibly important among bio-medical implants because of their high strength and resistance to fatigue deterioration. Recently, the development of non-toxic, more biocompatible and allergy-free components has been of outmost importance. The purpose of this study was to use first principle approach to investigate the effect of alloying Ti with Nb and Zr to improve the mechanical properties of Ti alloys for use in human implantations. This is attributed to the β phase stabilization ability and high bio compatibility of these transitional element. Increasing Zr and Nb concentrations on the Ti stabilized the alloy with a lower young's modulus compared to that of pure Ti.

Key words: Titanium alloys, Heats of formation, Lattice parameters, Density of states, Elastic properties.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

Hons

Photonics / **306**

The Uncertainty Principle with a Twist

Author: Neelan Gounden[1]

Co-authors: Isaac Nape [2]; Geoff Beck [1]; Andrew Forbes [3]; Jenna Epstein [1]

[1] *University of Witwatersrand*

[2] *Structured Light Lab, School of Physics, University of Witwatersrand*

[3] *U. Witwatersrand*

Corresponding Author: 2097061@students.wits.ac.za

Karl Popper, a philosopher, had found the entanglement of particles fascinating. He wanted to test the standard interpretation of quantum mechanics since he believed that knowledge of one of the entangled particles should not affect the properties of the other entangled particle, as well as investigating the presence of a non-local influence in these systems. The behaviour of a quantum entangled particle passing through a physical slit differs from that of a quantum entangled particle passing through a virtual/ghost slit. For an entangled particle passing through a slit of an infinitesimally narrow width, it would be predicted by the Copenhagen interpretation of quantum mechanics that the uncertainty in momentum will approach an unbounded value. I will present the experiment which we conducted whereby the vertical slits are replaced by angular slits and orbital angular momentum is measured instead of linear momentum. It can be concluded from the results that an entangled particle passing through an infinitesimally narrow slit has its momentum spread being limited by the initial momentum produced by the source.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / **307**

Linking Quantum Search Algorithms to Ghost Imaging

Author: Neelan Gounden[1]

Co-authors: Paola Concha Obando [2]; Isaac Nape [3]; Andrew Forbes [4]

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[2] *Wits University*

[3] *Structured Light Lab, School of Physics, University of Witwatersrand*

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Corresponding Author: 2097061@students.wits.ac.za

Ghost imaging is the process of reconstructing an image of an object using entangled photons. One of the entangled photons interacts with the object and is detected without spatial resolution while the other photon from the pair is detected with spatial resolution. When the two photons are detected in coincidence, an image of the object can be obtained with the help of projective masks. An analogy can be drawn between the Grovers algorithm (quantum search algorithm) and the detection of single photons to produce a ghost image of a given object. The Grover operator (consisting of the oracle and the diffuser) contains similarities to the operator which acts on the projective states in the ghost imaging procedure. This correlation presents a new method of performing ghost imaging. I will present our findings as to how Grover's algorithm is linked to bi-photon detection and how Grover's operator emerges.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Photonics / 308

Studying quantum-like light from simple laser systems

Author: Light Mkhumbuza[None]

Co-author: Andrew Forbes [1]

[1] *U. Witwatersrand*

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In the extremes of quantum and classical states of light we find quantum-like light, coherent states that look like particles but behave like waves. Here we present a novel laser that exhibits quantum (wave) and ray (particle) like features. We build the laser cavity using simple linear optical elements and show that the relation between the cavity length(L) and radius of curvature(R) when precisely controlled determines different periodic oscillating ray trajectories in the cavity with different longitudinal frequency modes. We also exploit the use of an off-axis pump laser diode to pump different positions of the crystal attached to the flat mirror to generate arbitrary oscillating ray patterns in the stable plano-concave resonator to illustrate the concept of ray-wave duality.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / 309

Structural, elastic, electronic, bonding, and optical properties of PtBiTe and PtBi₂ structures.

Authors: Masilu Godfrey Mulaudzi[1]; Thamari Dlamini[None]; Phuti Ngoepe[1]

Co-author: Bradley Nemutudi [1]

[1] *University of Limpopo*

Corresponding Author: godfrey.mulaudzi@ul.ac.za

In recent days, semimetals have become an active branch of materials research. The Platinum Group Mineral (PGM) semimetal Insizwaite (PtBi₂) and Maslovite (PtBiTe) are polymorphic systems with interesting electronic properties. Here we report the optimised crystals belonging to the pyrite-type cubic structure which are important electronic systems to investigate both from the point of view of fundamental physics and prospective applications. We have employed the density functional theory (DFT) to investigate the structural, elastic, mechanical, electronic, bonding and optical properties of PtBi₂ and PtBiTe.
Calculations of elastic constants and moduli indicated that PtBi₂ and PtBiTe possess a low level of elastic anisotropy, reasonably good machinability, mixed bonding characteristics with ionic and covalent contributions, brittle nature and relatively high Vickers hardness with a low Debye temperature. The mechanical stability conditions were fulfilled. Analysis of bond population supported the bonding nature as indicated by the elastic parameters. The bulk electronic band structure revealed clear semi-metallic features with signature Dirac cone-like dispersions near the Fermi level. A pseudo gap in the electronic energy density of states at the Fermi level separating

the bonding and the antibonding peaks point towards significant electronic stability of cubic of PtBi₂ and PtBiTe. The Fermi surface mostly consisted of electron-like sheets with very few small hole pockets. The band structures were isotropic in the k-space. The optical constants indicated interesting characteristics. Furthermore, all the energy-dependent optical parameters exhibited clear metallic signatures and were in complete accord with the underlying bulk electronic density of states calculations. we calculate the electronic band structure using the obtained structure parameters. These findings warrant further research using a broader array of experimental techniques.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / 310

Synthesis and Characterization of Ti3C2 MXene electrode via In-situ HF and direct HF etching methods for application in battery-supercapacitor hybrid devices.

Authors: Tsholo Talane[1]; Bakang Moses Mothudi[2]; Katlego Makgopa[1]; Mokhotjwa Simon Dhlamini[2]

[1] *TUT*

[2] *University of South Africa*

Corresponding Author: talanete@tut.ac.za

The need for cleaner, renewable energy to tackle issues such as global warming and the rapid consumption of fossil fuels has led to an increased interest in developing high-energy and high-power density energy-storage devices. While batteries were extensively used for energy storage in the past, they suffer from a limited number of charge cycles and longer recharge times. Electrochemical capacitors have high power provision but possess comparatively low energy density. To mitigate this, a hybrid solution combining battery and supercapacitor electrochemical performance is necessary.

Herein, we report on the fabrication and structural optimization of a Ti3C2 MXene pseudo-capacitive electrode via In-situ HF and direct HF etching of the Ti3AlC2 MAX phase for use in battery-supercapacitor hybrid devices.

The SEM results showed a stacked multilayer with highly delaminated morphology, clearly exhibiting significant openings of the MXene lamellas. The EDX analysis confirmed that the MXene sample has a lower percentage of Al element; 0.78% and 0.59% for direct HF and In-situ method respectively compared to the as-prepared MAX sample (12.72%). This indicates successful etching of the Al element from the precursor sample. However, EDX showed small traces of F and Cl elements in samples synthesized using the in-situ method; a clear indication that this method requires further treatment with chemical substances such as NH4HF2 and NH4F for complete HCl etching. From the XRD pattern, the eradication of (104) peak at ˜39.0˚ 2θ for all samples indicates the full conversion of Ti3AlC2 to Ti3C2, with no notable impurity signals as seen on the EDX data, further cementing the SEM and EDX analyses.

The electrochemical properties of the MXenes are discussed, followed by their application in various fields of the energy storage industry, especially in multifunction electronics, hybrid electric vehicles, and industrial equipment.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / 311

Fitting NOvA and T2K data with the revamped A_4 symmetry model for the poorly constrained neutrino oscillation parameters

Author: Thabo Msiza[None]

Co-authors: Soebur Razzaque [1]; Ushak Rahaman [1]

[1] *University of Johannesburg*

Corresponding Author: thabowonderbymsiza@gmail.com

The Standard Model is widely accepted as one of the most successful predictive theories of Physics, providing insight into the fundamental building blocks of the universe. Over the last few decades this model has shown signs of incompleteness, most of which are attributed to Neutrinos. Within the confines of the standard model a discrepancy exists related to vanishing Neutrino masses, which contradicts the experimental observation of Neutrino Oscillation. Neutrino oscillation depends on 7 parameters (3 mixing angles $\theta_{12}, \theta_{23}, \theta_{13}$, a Dirac Phase due to CP violation δ_{CP}, and the 3 mass states m_1, m_2, m_3). Values of the parameters θ_{12}, θ_{13}, Δm^2_{21}, $|\Delta m^2_{32}|$ are well determined whilst θ_{23}, δ_{CP} and the mass Hierarchy, whether ($m_1 < m_2 < m_3$) or ($m_3 < m_1 < m_2$), remain poorly determined. The goal of this research is to make use of the Revamped BMV (Babu-Ma-Valle) model to attempt a constrain of the poorly determined parameter values of δ_{CP} and θ_{23} using data from the NOvA and T2K experiments. We identify how the current Standard Model constraints the aforementioned parameters so as to have a comparative analysis of the constraining ability of both models. The analysis of $\Delta\chi^2(\theta_{23}, \delta_{CP})$ suggest better constraints can be obtained for the NOvA experiment in 3σ region, the T2K experiment has no visible difference in both models. The combined (NOvA+T2K) analysis is driven by the new model's effect on the NOvA data. The model fundamentally constraints the poorly determined parameters the same way, with the only exception being in the 3σ region.

Apply to be considered for a student ; award (Yes / No)?:

YES

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / 312

Characterization of neutron-induced defects in SnO2 using positron annihilation technique

Author: Dineo Motjope[None]

Co-authors: L Ngwazi ; M Madhuku ; Phumlani Zipho Ngcobo [1]; T Jili

[1] *University of Zululand*

Corresponding Author: dineopatience02@gmail.com

In this work a two-component density functional theory is employed in the modelling of defects in neutron-irradiated SnO2. Since defects are localized, the local density approximation (LDA) is used which is part of DFT. Although LDA gives a good approximation of positron lifetimes and electron-positron annihilation momentum density, it does not consider the variation nature of the electron density. This has an unintended consequence of having over estimated annihilation rates or lower positron lifetimes compared to experimental values. This deficiency in LDA is corrected by using the generalized gradient approximation (GGA) which considers the variation nature of electron density. The accumulation of annihilation spectrum using coincidence setup, is utilized to allow for the determination of annihilation parameters, S and W. The spectrum consists of positron annihilations at defect sites as well as annihilations in the bulk (defect-free region). It also consists of annihilations of positrons with core electrons (high momentum electrons). The low and high momentum distribution of electrons will be used to characterize the Doppler broadening which will tell us about the quantity of radiation-induced defects in SnO2 in terms of calculating S-parameter, which is the ratio of the annihilation centroid area to the total area of the annihilation curve. Calculated S parameters are then compared with the experimentally obtained S parameters. The nature of the defects is theoretically obtained from the annihilation rates or equivalently from the calculated positron lifetimes in SnO2.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Nuclear, Particle and Radiation Physics / **313**

Machine Learning-based Gamma Spectroscopy with Multi-Spectral Tracking

Authors: Shaun Wyngaardt[1]; Calib Buckton[1]; Mkhuseli Nqxande[1]

[1] *Stellenbosch University*

Corresponding Author: 19825706@sun.ac.za

This project entails the development of a machine learning-based gamma detection system with tracking and prediction capabilities. It involves integrating gamma spectroscopy via an artificial intelligence model, including a custom neural network trained on spectra from various isotopes and a compact detector. The model would be integrated into a compact, low-cost, micro-controller enabled system with additional sensors to provide the hardware. This includes, but is not limited to, a thermal sensor, GPS sensor, multi-spectral camera, etc. and would be used to run and manage the model. The overall system with the neural network and multi-spectral system would be designed to provide a useful and inexpensive complement to current radiation safety methods and additionally serve as an early warning system (e.g. in the case of radiation leaks). Additionally, the treatment of noise in the obtained spectra, both environmental and systematic, will be investigated in this research via neural networks and Kalman filters. This is crucial for monitoring out in the field, where low-level monitoring often suffers from background interference. The value is increased by the packaging of thermal and GPS sensors, together with a standard camera and infrared camera for mobile object detection, complementing the gamma-ray spectra identification.

Thermal sensors combined with an infrared camera can allow the detection of heat signatures, which is useful for finding the source of emissions. Through the use of recursive

algorithms, an interactive multiple-model estimator could offer prediction capabilities through modelling trajectories of
gamma radiation within the environment. Eventually, a self-correcting system with identification and tracking can be used to
provide early warning or other useful information regarding radiation in the environment. Although a stationary system with stationary sources will be tested, one could easily apply this to a dynamic mobile system (e.g. drones and surveillance cameras) with the addition of motors or compact vehicles for transportation. This system could be compared to existing radiation safety methods and warning systems, as well as machine learning benchmarks for spectra prediction. For example, one could test how well it identifies radiation leaks, the number of false positives, and the accuracy of the tracking system.

It is also believed that the supervised training process of the
network can include examples of noise, to assist in obtaining as clean a spectrum as possible, and to guide the network to the true reaction data.
Ideally, the network will learn to identify the isotopes by peaks and possibly backscatter patterns. This will prevent the inclusion of unanticipated sources confusing the network when making predictions.

The consideration of radiation monitoring environments, such as nuclear waste disposal sites and nuclear power plants (e.g. Koeberg), yields insights to the value of this research. A low-cost, efficient radiation monitoring device could assist in radiation protection cases, capable of detecting gamma emissions and hotspots in the surrounding environment. There is also the use in the field, for remote monitoring and built-in GPS for localization. Moreover, a mobile system can be used to investigate stationary and moving
5
sources in the field (e.g. geological vaults), providing information regarding the energies and intensities of various gamma sources. There is also the knowledge gained by investigating further development of micro-
controller-enabled systems with deep learning-based object recognition and tracking software. There is a direct comparison to be made with existing surveillance and monitoring technology.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Photonics / **314**

Investigating mode diversity with combinations of Hermite-Gaussian and Orbital Angular Momentum modes

Author: Alice Drozdov[None]

Co-author: Mitchell Cox [1]

[1] *University of the Witwatersrand*

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Free space optical communication has the potential to mitigate the existing digital divide. However, it is highly susceptible to atmospheric turbulence, especially when used with mode division multiplexing. Turbulence decreases the received power of the transmitted laser beam, thus inducing errors. By simultaneously transmitting and/or receiving two modes, the received power could be

improved. This method, known as mode diversity, has been shown to improve error rates in systems. Previous studies have primarily focused on Orbital Angular Momentum (OAM) modes, but other mode combinations, such as two Hermite-Gaussian (HG) modes or even a combination of an OAM mode and an HG mode, could also be utilized. In this work, we investigate the received power of a system using mode diversity with various mode combinations, including two OAM modes, two HG modes, and an HG and OAM mode, in the presence of real atmospheric turbulence.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / **315**

Exploring dark Z_d-boson at LHC

Authors: Karabo Mosala[1]; Mukesh Kumar[1]; Kumar Setendra[2]

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Hidden sectors or dark sectors are hypothetical components appearing in various extensions to the Standard Model (SM), introduced to address phenomena not addressed by the SM (e.g the existence of dark matter or positron excess in the cosmic microwave background radiation flux). To incorporate the hidden sector, the introduction of an additional $U(1)_d$ dark gauge symmetry is necessary. This implies the presence of an extra gauge boson, often referred to as a dark photon or dark gauge boson Z_d^μ. The dark photon could interact with both the hidden sector particles and the SM particles through a kinetic mixing term. The coupling between the dark photon and the SM can be explored at the Large Hadron Collider (LHC) through proton-proton collisions. We probe various possible channels in the LHC environment and study the constraint on coupling(s) versus m_{Z_d} at the centre of mass energy $\sqrt{s} = 13.6$˜TeV with expected luminosity.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Photonics / **316**

Beyond doughnuts and mugs, tying photons together

Authors: Pedro Ornelas[1]; Isaac Nape[2]; Robert De Mello Koch[3]; Andrew Forbes[4]

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[2] *Structured Light Lab, School of Physics, University of Witwatersrand*

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Entanglement between photons has been a source of great interest in the past few decades being the catalyst for fundamental tests of quantum mechanics and offering a plethora of applications from ghost imaging to quantum key distribution. However, these entangled photon states are highly susceptible to environmental disturbances, thus requiring mechanisms for robustness in harsher environments. Topology is capable of providing these mechanisms, rejecting such disturbances entirely by characterizing systems according to an invariant property of the system, universally named its topological charge. An interesting topology is that of the skyrmion which has proven to be highly versatile, manifesting in spintronics, condensed matter physics and more recently optics. Here we report the first non-local quantum skyrmion whose topology can be controlled directly through control of its non-separable, biphoton wavefunction. We discuss a new classification mechanism where wavefunctions are distinguished according to their topology. We further demonstrate that the topology of the wavefunction persists even when entanglement is fragile.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics of Condensed Matter and Materials Track 2 / 317

Emulating magnetic skyrmions with light

Authors: Pedro Ornelas[1]; Keshaan Singh[1]; Angela Dudley[2]; Andrew Forbes[3]

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Magnetic skyrmions are topologically stable spin systems that cannot be smoothly deformed into any other spin configuration that differs topologically or possesses a different integer topological invariant, the Skyrme number. Their robustness has generated interest in using them as a resource for low power, information storage and computing. Recently topologically equivalent configurations have been generated in optical systems using structured light techniques. Here, we introduce an optical analogy to magnetic skyrmion dynamics subject to a magnetic field. Our optical skyrmions are engineered using superpositions of Bessel-Gaussian beams, with propagation dynamics mimicking the temporal evolution of their magnetic counterparts. We show that whilst the topology remains invariant, the texture of the optical configuration changes during propagation, exhibiting controllable periodic precession over a well-defined range, analogous to time varying spin precession in homogeneous magnetic fields. Furthermore, we discuss a general technique to control the on-axis optical spin to emulate any given magnetic spin subject to an arbitrary magnetic field. We believe this work offers new tools to study magnetic skyrmion dynamics subject to applied magnetic fields.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Theoretical and Computational Physics / 318

Non-local topological rejection of noise

Authors: Pedro Ornelas[1]; Isaac Nape[2]; Robert De Mello Koch[3]; Andrew Forbes[4]

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Corresponding Author: 1836488@students.wits.ac.za

Topological properties of physical systems have been studied for many years for their robustness against environmental disturbances which leave these properties unchanged. In the context of magnetic systems, a topology that has been extensively investigated is that of the skyrmion where it has been shown to provide some utility for use in low-power, information storage and computing. More recently, the optical analogy to these systems has been studied in classical beams with inhomogeneous polarization structures. Here we show the first non-local realization of the skyrmionic topology manifesting as a shared property between two entangled photons. Furthermore, we explore the topological robustness of these entangled states to channels which decay its degree of entanglement as well as those which add in isotropic noise into the system. We then present simple arguments to explain how the topological noise rejection works in each case. We believe this work reveals a deeper connection between topology and entanglement and offers a new mechanism for constructing more robust quantum states.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / 319

Li adsorption on a self-healed graphane for the next generation ion batteries.

Authors: Edwin Mapasha[1]; Igumbor Emmanuel [2]; Kgalema Phodisho [3]

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[2] *University of Johannesburg*

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Density functional theory calculations were performed to study the behaviour of Li atom on self-healed various CH divacancies graphane focusing on the reconstructed lattices. The energetic stability, structural and electronic properties of different Li configurations on self constructed topological 5-9-5 and 9-5-9 defects were examined. These lithiated configurations have high binding energy significantly more than that of Li on graphene and bulk metalic lithium, suggesting a plausible materials for experimental characterizations. All the lithiated configurations relaxes towards the vacancy with 5-9-5 defect having a 0.00 Å height. The Li atom introduces delocalised states within the band gap, exhibits metallic character with considerable electronic states at the Fermi level, which can provide good electrical conductivity during the battery cycle. These results suggest that Li configurations on self constructed topological 5-9-5 and 9-5-9 defects can be utilized as a promising anode material for the application in Li ion batteries with fast charge/discharge rates.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Photonics / **320**

Threading a Laser Through the Eye of a Needle 2.0: Evaluating Coupling Performance of Telecom Fibre Cables for use in a Cost-Effective Free Space Optical (FSO) System under Atmospheric Turbulence.

Author: Fortune Iga[1]

Co-author: Mitchell A. Cox [2]

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This research is dedicated to the development of a cost-effective Free Space Optical (FSO) system using standard telecom fibre cables. These cables, which include the single-mode and five multi-mode fibre cables (OM1, OM2, OM3, OM4, and OM5), are selected for their wide availability and cost-effectiveness. This study assesses the coupling performance of these fibre cables in the presence of atmospheric turbulence, by subjecting them to controlled turbulence effects using a spatial light modulator (SLM). Key turbulence effects such as beam wander, angle of arrival fluctuations, spatial coherence loss, and scintillation are analysed. The findings of this research contribute to the advancement of an accessible FSO system capable of providing connectivity prior to fibre cable installation, thereby playing a crucial role in bridging the digital divide.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / **321**

Analysis of green emitting Tb3+ activated BaAl2O4 /CaAl2O4/AlHO2/ Tb2O3/TbAlO3 mixed phases nanophosphors prepared via citrate sol-gel method

Authors: ABONGILE BELE[1]; Motlalepula Rebecca Mhlongo[2]; Lehlohonolo Koao[3]; Setumo Victor Motloung[4]

Co-author: Tshwafo Motaung [5]

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[2] *Sefako Makgatho Health Sciences University*

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BaAl2O4 /CaAl2O4/AlHO2/Tb2O3/TbAlO3:x% Tb3+ ($0 \leq x \leq 1.9$) mixed phases nanophosphors were developed using sol-gel synthesis. The phase quantification of the XRD results indicated that the mixed phases are composed of the hexagonal (BaAl2O4, CaAl2O4), orthorhombic (AlHO2, TbAlO3) and cubic (Tb2O3) crystal structures. SEM results showed the presence of the nano which enlarged with the increase in Tb3+ concentration. TEM confirmed the presence of nanorods. Photoluminescence (PL) results depict emission peaks at 380, 415, 435, 458, 488, 542, 586 and 622 nm attributed to 4f–4f Tb3+ transitions 5D3⟶7F6, 5D3⟶7F5, 5D3⟶7F4, 5D3⟶7F3, 5D4⟶7F6, 5D4⟶7F5, 5D4⟶7F4, and 5D4⟶7F3, respectively. Commission Internationale de l'éclairage (CIE) shows that the Tb3+ doped samples emitted the green colour

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Applied Physics / 322

The varying and invariant properties of vectorial light for robust communication through a 270m free space optical link with no pre- or post-correction

Authors: Cade Ribeiro Peters[1]; Mitchell A. Cox[2]; Alice Drozdov[None]; Andrew Forbes[3]

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Vectorial structured light has found numerous applications due to its unique properties and has many advantages over scalar light fields. However, there has been a lot of debate regarding the robustness of these modes to certain aberrations and distortions which has significant implications for the uses of these forms of light, including for communications, imaging and sensing. In this work examine the behaviour of vectorial light through the dynamic and highly aberrated medium of atmospheric turbulence using a real-world 270m free space optical link. We definitively show the amplitude, phase and polarisation distortions induced by the medium. We present the first ever experimental demonstration of the invariance of the concurrence (a quantity that measures the non-separability and variations in the beam's polarisation structure) through real-world atmospheric turbulence. Such a quantity allows for the encoding of information without the need for a shared basis and requires no error correction and thus holds many advantages over alternative means of communication. The invariance holds for multiple beam types over long periods of time through the dynamically changing medium and through various degrees of distortions induced by the atmosphere. The results of this work are therefore highly interesting for the use of vectorial light through various, complex media and for both classical and quantum communications and imaging.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Photonics / 323

Uncovering the spatial distribution of entanglement using vectorial light

Authors: Cade Ribeiro Peters[1]; Andrew Forbes[2]

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Vectorial light has long been established as a robust analogy for 2-dimensional quantum systems. Consequently, many of the insights and techniques from quantum mechanics, and entanglement in particular, have found significant applications in helping us understand and quantify many properties of vectorial light. This relationship also allows us to probe the nature of quantum systems using vector modes. Traditionally the degree of entanglement of a quantum state is thought of as a single value between 0 and 1. In this work we use the non-separability of vectorial light as an analogy for the degree of quantum entanglement and show that this value does not just vary between 0 and 1, but also changes depending on where in the state one chooses to look. Thus entanglement is not just a global property of the system, but varies spatially across the entire state. The results of this have applications in the fields of quantum imaging and allow for more detailed investigations of how entanglement evolves in complex quantum systems.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 2 / 324

Achieving reliable and robust optical communication through a change of basis

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Free space optical communication has proven to be an effective form of transmitting information over large distances. Structured light has proven to be a valuable tool in improving such channels but is quickly reaching its limits due to the distortions induced by atmospheric turbulence. It has been shown that certain shapes of light, the eigenmodes of turbulence, remain invariant to these effects and can pass through the atmosphere unaffected. However, current methods produce eigenmodes that are not always viable to generate for real world use, lack an analytical description and are ineffective in practical applications. In this work we put forward a new method for calculating these eigenmodes by using an operator in the OAM basis. This basis is chosen because it is complete, meaning any light field can be decomposed into a superposition of OAM modes, and because these modes show low divergence in the paraxial regime. The new operator is found by first defining

the transformations in the position basis and then decomposing this operator into the OAM basis. This has numerous benefits over previous approaches as it provides an analytical description of these eigenmodes, gives us insight to their propagation dynamics and relationship to the channel distortions and most importantly outputs modes that are reliably robust through turbulence. These results are not only of interest to the field of communications, but will also have applications to imaging, sensing and quantum optics.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Nuclear, Particle and Radiation Physics / **325**

Refurbishment of the SK solenoid magnetic lens spectrometer at iThemba LABS

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Co-authors: Pete Jones [2]; Abraham Avaa [3]; Richard Newman [4]; Lumkile Msebi [5]

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A solenoid magnetic lens spectrometer \cite{avaa2020electron} was refurbished and upgraded to incorporate measurement of internal-pairs in addition to conversion electrons. An in-beam experiment was performed on a setup where the magnetic lens spectrometer was coupled to a gamma-ray array consisting of seven Compton suppressed HPGe clover detectors. A 1.1 mg/cm^2 thick ^{50}Ti target was bombarded with a 30 MeV alpha beam \cite{oakley1987pion}\cite{pronko1974gamma}\cite{morsch1973monopo in an attempt to excite the 0^+ state at 3.8 MeV, which is expected to subsequently decay via internal-pair formation. The populated nuclei were identified and the observed gamma-ray transitions were built into level schemes. A thorough investigation of gamma-internal-pair and gamma-conversion electron coincidence was also carried out both for a radioactive source (^{207}Bi) and in-beam data. This study highlights the unique capability of of the solenoid magnetic lens spectrometer in measurements of electric monopole ($E0$: $0^+ \rightarrow 0^+$ or $J^\pi \rightarrow J^\pi$) transitions, the only significant alternative nuclei decay mode in cases where nuclear decay via gamma-ray emission is forbidden \cite{ANAndreyev}\cite{wood1992coexistence}\cite{kibedi2005electric}\cite{wood1999electric}.

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / **326**

A study of thermal response of chromium-tin (Cr-Sn) bimetal films using in-situ RBS by Artificial Neural Networks

Authors: Ingrid Segola[1]; Christopher Mtshali[2]; Lebogang Kotsedi[2]; Mandla Msimanga[3]

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Bimetallic thin films of chromium-tin (Cr-Sn) were prepared using electron beam evaporator, the films were prepared such that a layer of chromium was deposited onto a thin film of tin. The first sample was then annealed in the Rutherford Backscattering Spectrometry (RBS) chamber under high vacuum, while probing with alpha particles. The RBS spectra were collected in-situ while annealing at a ramp rate of 3℃/min, from room temperature to 600℃. A 2 MeV He^{2+} ion beam was used to probe the sample for atomic depth profiling evolution. The collected spectra were analysed using Artificial Neural Networks (ANNs). The ANN model was trained using a set of simulated RBS spectra generated using the SIMNRA software package. The results of stochiometric analysis showed that the layers of Cr-Sn start phase changing at temperatures of ~275℃ and ~475℃ for the CrSn and Cr_2Sn phases respectively.
The second sample was heated using femtosecond laser with the wavelength of 1064 nm, and a pulse duration of 190 fs, with the repetition rate of 200 kHz, the net-fluence used were ranging from 300 J/cm^2 to 970 J/cm^2. The two-temperature model was performed using the finite element method to study the thermal behaviour of the films, the results revealed that the films absorbed the laser heat within a few picoseconds. The results of this study demonstrate the potential of ANNs in the analysis of RBS spectra and the importance of considering the thermal effects during thermal treatment.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 1 / 327

Magnesium-Silicon Alloy Phase Stability Predictions: A cluster expansion study.

Authors: Kgotso Chuene[1]; Katlego Phoshoko[1]; Phuti Ngoepe[1]

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Rechargeable batteries have the potential to help meet the ongoing demand for portable energy and to mitigate the energy crisis in countries such as South Africa. These call for the accelerated development of novel and advanced high-energy battery electrode materials. Magnesium-Silicon (Mg-Si) anodes have emerged as attractive alternatives to the graphitic anodes used in current lithium-ion battery technologies. However, the commercialisation of batteries based on the Mg-Si alloy is deterred by a few obstacles including the incompatibility of the Mg-Si anode with conventional battery electrolytes. In this work, the material space of the Mg-Si alloy system was explored through crystal structure predictions conducted via a machine learning (ML) powered cluster expansion technique (CE). The aim was to predict and analyse novel and stable phases of the magnesium-silicon alloy system whose compatibility with electrolytes shall be interrogated in future work. The genetic algorithm embedded within the CE technique was used to accelerate the material discovery

process by performing the ground-state search of stable structures from the Mg-Si alloy system. By considering the BCC and FCC-based parent lattice, 8 structures were predicted to be thermodynamically stable, namely, Mg₅Si (Imma), Mg₂Si (P-3m1), MgSi (P4-mmm), Mg₃Si (Pm-3m), MgSi₃ (Pm-3m), MgSi₃ (P2-m), MgSi (Im-3m), and Mg₃Si (P4/mmm). The geometric properties of these structures are presented. From the predicted structures, the orthorhombic magnesium-rich phase, Mg₅Si, was found to be structurally stable and a promising candidate for Mg-Si-based rechargeable batteries. The findings from this study are crucial to the advancement of high-energy battery electrode materials for next-generation batteries.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 2 / 328

Comparison of A12O3 and Fe2O3 surfaces using First Principle method

Authors: Mpho Enoch Sithole[1]; Patricia Dibakwana[None]; Rosinah Modiba[None]; Tshwane David [None]

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Comparison of A12O3 and Fe2O3 surfaces using First Principle method

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ABSTRACT
Al2O3 and Fe2O3 are oxide materials that are widely used in a variety of applications, including catalysis, ceramic-based semiconductors, corrosion protection, and thermal barrier coatings. However, most of the material strength applications depend on its surface properties. The purpose of the study was to investigate the structural. In this study First Principle calculations based on density functional theory were performed with Cambridge Serial Total Energy to investigate the surface stability between Al2O3 and Fe2O3 surfaces.
The results show that the surface energy of Al2O3 is lower than that of Fe2O3 in all three planes. Therefore, the surface energy values of Al2O3 increase in this order 100< 111<110 Al2O3 and for Fe2O3 it increases in this order 111<110<100, which explains that the 100 plane has the lowest surface energy for Al2O3 and 111 has the lowest surface energy for Fe2O3 The results suggest that Al2O3 is more stable and energetically favorable, since it exhibits a low surface energy on all planes than Fe2O3surfaces. In addition, partial density of states and work function were computed and analyzed.

Keyword: Oxide materials, First principle, Millar index, Aluminum oxide, Iron oxide

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Poster Session 1 / **329**

Optimization of electron transport layer in polymer solar cell

Author: Modisa Ntobeng[None]

Co-authors: Thapelo Seimela [1]; Nolwazi Nombona [2]; Mmantsae Diale [3]

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[2] *University of pretoria*

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Organic solar cells (OSC) will soon be commercialized because of their benefits such as low cost, light-weight, flexibility, and the ability to process for very wide area applications. Polymer semiconductors may have the potential to replace silicon in next-generation solar cells. Despite these benefits, there is still some room for improvement in polymer solar cells power-conversion efficiency (PCE), which is crucial for their commercialization. High device efficiency and stability depend on the interlayers between the photoactive film and the electrodes. Therefore, in this study we compared the stability and performance of indium tin oxide (ITO) substrate with that of membrane substrate. The structure, morphology and electro-optical characteristics of the ITO substrate and membrane substrate samples have been analyzed by different characterization techniques such as X-ray diffraction (XRD), scanning electron microscope (SEM) and ultraviolet visible spectroscopy (UV-vis).

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics of Condensed Matter and Materials Track 2 / **330**

Magnetic properties of Cr doped CoV2O6: A binary phase study

Authors: Murei Mulibana[1]; Pankaj Mohanty[1]; Aletta Prinsloo[1]; Charles Sheppard[2]; Bincy Susan Jacobs[3]

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The one-dimensional spin chain system CoV2O6 is known to show unique magnetic properties such as metamagnetism characterized by a 1/3 magnetic plateau [1–3], and magnetocaloric properties [3].

CoV2O6 crystallizes in two structurally distinct but chemically identically phases, α–CoV2O6 and γ–CoV2O6. Several studies have explored the magnetic properties of these two phases in bulk single crystalline [1,4] and polycrystalline [2,3] as well as nanocrystalline samples [5,6]. Recently, the effects of Cr doping on the magnetic properties of α–CoV2O6 were explored [7] and the study revealed the presence of spin-glass-like behaviour in addition to metamagnetism. This study takes an innovative approach of investigating the magnetic properties of a binary phase Co(V0.90Cr0.10)2O6 sample. The sample was synthesized using a wet chemical synthesis method [7]. The structural, elemental, morphological and magnetic properties of Co(V0.90Cr0.10)2O6 were investigated using X-ray diffraction (XRD), energy dispersive X-ray spectroscopy (EDS), Scanning electron microscopy (SEM), and vibrating sample magnetometry (VSM), respectively. XRD data revealed that Co(V0.90Cr0.10)2O6 sample is a binary phase of α–CoV2O6 and γ–CoV2O6. Rietveld refinement was performed on the XRD data and revealed that the composition consists of 84.90 % α–CoV2O6 and 15.10 % γ–CoV2O6. The calculated lattice parameters for both phases are in good agreement with those reported by Nandi and Mandal [3]. EDS elemental spectra showed the presence of Co, V, Cr and O, indicating the elemental purity of the samples and demonstrating the successful doping of Cr in the CoV2O6 matrix. SEM analysis revealed that the prepared powder sample is made of particles of different morphologies. The magnetic properties of Co(V0.90Cr0.10)2O6 were probed by measuring the magnetization as a function of temperature, M(T), under zero-field-cooled (ZFC) and field-cooled (FC) protocols at 0.1 T, 2.5 T and 5 T. M(T) data at 0.1 T reveals an antiferromagnetic (AFM) ordering with ordering temperature, TN = 15.2 ± 0.3 K. Increasing field to 2.5 T results in a ferrimagnetic (FI)-like ordering with TN = 13.3 ± 0.2 K. Increasing the field strength to 5 T results in a ferromagnetic ordering with TN = 15.2 ± 0.2 K. Spin-glass-like freezing was observed at 2.5 T. Isothermal field dependence of magnetization, M(μ0H), measurements at 2 K, 5 K, and 7 K, show a stepwise dependence of magnetization on the applied field, known as metamagnetism, with the first, second and third step corresponding to AFM, FI, and FM ordering, respectively. Metamagnetic transitions occurs at critical fields Hc1 and Hc2, with Hc2 ≈ 2Hc1. Finally, magnetic saturation occurs at the FM state, with the values of saturation magnetization, Ms, smaller than those of α–CoV2O6 and larger than those of γ–CoV2O6 [2], demonstrating the binary nature of Co(V0.90Cr0.10)2O6. The results from this study will contribute significantly to the existing knowledge of the magnetic properties of CoV2O6 and potential application in technology.

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[7] M. Mulibana et al., AIP Adv. 13, (2023).

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Physics for Development, Education and Outreach / 331

The need for an integrated approach to physics/science capacity building in South Africa, SADC region, and Africa

Author: Azwinndini Muronga[1]

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Globally, several countries/regions have been busy strategizing around their physics visions for the next decade or so. The African continent has also started with a similar journey.

In this talk I will present the current international efforts as well as the initiatives in Africa regarding vision(s) for physics. I will focus on the issues of (i) diversity, equity, and inclusion in physics/science capacity building, (ii) education and outreach or science engagement for physics/science capacity building, and (iii) initiatives in physics/science graduate/postgraduate capacity building.

I will then highlight the need for an integrated approach to the value chain of physics/science capacity building.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Applied Physics / **332**

Button Optics: On-demand generation and diagnosis of structured light

Authors: Bertus Jordaan[1]; Keshaan Singh[1]; Angela Dudley[1]; Andrew Forbes[2]

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Understanding and controlling structured light has led to many exciting opportunities in physics, optics, biophysical and related research fields. However, the required technical knowledge to use this promising technology remains an obstacle for non-experts. At Button Optics, we provide turnkey solutions that use digital technology to generate and diagnose structured light. We briefly present the underlying physics and technology and showcase the current state-of-the-art capabilities of our prototype.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Applied Physics / **333**

Severe Accident Analysis at Koeberg Nuclear Power Station Using MELCOR Computer Code

Author: Nontobeko Khumalo[1]

Co-authors: Bonginkosi Mnisi [1]; Ian Korir [1]

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In the demonstration of safety of a nuclear power plant (NPP), simulations for all plant states (normal operations, anticipated operational occurrences, design-basis accident, and beyond-design-basis accident) play an important role. Therefore, computer codes have been extensively developed to analyse the different aspects of a nuclear reactor. Thermo-hydraulic system codes are used to study the physical response of the reactor system to postulated transient and accidental events and determine if any failure may lead to a significant release of radioactivity.
MELCOR (Methods for Estimation of Leakages and Consequences of Releases) is one of the codes that can be used for severe accident analysis. Other codes like MAAP (Modular Accident Analysis Program) and ASTEC (Accident Source Term Evaluation Code) can also be used. MELCOR is a fully integrated, engineering-level computer code that models the progression of severe accidents in light water reactor nuclear power plants.

The National Nuclear Regulator (NNR) is developing a computer model of Koeberg Nuclear Power Station (NPS) to be used for severe accident analysis of the plant. This work enables the NNR to independently verify the severe accident analysis submitted by Eskom and ultimately verify if the accident management plans submitted by Eskom are effective. This work will also contribute to the review and assessment of the Koeberg long term operation (LTO) Safety Case submitted by Eskom for approval.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Theoretical and Computational Physics / 334

2022/2023 NMU-NITheCS Internship Programme: Connecting Quarks with the Cosmos, connecting people with the Universe

Authors: Azwinndini Muronga[1]; R. R. Baatjes[2]; B. Bhengu[3]; N. G. Cebekhulu[3]; K. Cele[4]; A. P. Dzhivhuho[5]; N. T. Gabela[3]; A. A. Guga[6]; B. V. Kamga[7]; T. C. Khumalo[8]; C. M. Machema[9]; V. Makumbane [10]; D. Mathebula[11]; Y. Mdlatu[12]; P. Mmatladi [6]; S. Mnisi[13]; A. M. M. Moeng[14]; M. M. Moila [15]; L. O. Mongale[9]; M. A. Mothibi[16]; D. P. Motjope[3]; S. H. Mthembu[2]; A. Mtuti[12]; S. Muronga[17]; T. E. Nemakhavhani [14]; P. Netshamutshedzi[18]; N. T. Netshiavha [6]; S. E. Netshiheni [5]; R. Netshikweta[19]; F. S. Nyaweni [12]; S. Ogundipe[3]; M. W. Paradza[20]; V. Phophi[5]; A. Qushu[2]; M. M. Ramaoka[21]; F. Raphulu[18]; M. M. Seabi[12]; M. Sibiya[2]; S. Somathube[22]; M. Thekhwe[21]; D. Worku[23]; S. Xipu[14]

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NMU-NITheCS Internship Programme is an annual summer study program in theoretical and computational sciences.
The internship research topics are under the overarching the subject: *Matter Under Extreme Conditions in Heavy Ion Collisions and Astrophysics* which is an inter-/trans-disciplinary subject as it is born at the borders between particle and nuclear physics, astrophysics, gravitation, and cosmology. This allows the collaboration of final year BSc, BSc (Honours), and MSc students from different disciplines such as mathematics, physics, statistics, and computing sciences to learn and to find solutions to cross-disciplinary scientific questions. The objectives of multiple disciplinary approaches are to resolve real world or complex problems, to provide different perspectives on problems, to create comprehensive research questions and to provide comprehensive solutions to the problems.

During the 2022/2023 NMU-NITheCS internship the interns had interactive sessions at Nelson Mandela University, Gqeberha from the 28th of November 2022 to the 23rd of December 2022. During the first two weeks of the internship the interns had an opportunity to attend the 7th Biennial African School of Physics (ASP2022) which was hosted at Nelson Mandela University in parallel with the internship. This was followed by 2 weeks of working on the assigned research topics to groups consisting of four interns per topic. The internship program then resumed online from mid-January 2023 to end of April 2023.

In this talk we will present the structure and processes of the internship programme as well as the overview of the results from each topical group and show the connections between topical groups as per the theme of the internship programme (title of the talk).

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Physics for Development, Education and Outreach / **335**

Decolonising the first year physics module at the University of Zululand.

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Reading the published paper claiming that Africans discovered gravitation before Newton, one begins to wonder. How many other discoveries have been taught in the universities that completely ignore the contribution of Africans in the discourse from ancient physics to modern physics. At

the University of Zululand (Unizulu), there is an emergence to include the African perspectives in our curriculum. This is work seeks to highlight and bring to the fore several physics concepts that dates back prehistoric times and are based on the ancient African civilisation as we know it. The theoretical formalism that underpins those concepts is investigated as well as their applications and recorded inventions in those times.

The units and measurements, the first chapter in the first-year physics module at Unizulu begins with the metric system which emerged in the 1900s and ignore the indigenous systems that Africans or any other civilization used before then. There were already standards that called for society to measure items for an example to achieve fair trade. In around 500BC the concept of time was already a subject of measurement because of empiricism that was prevalent as an approach to understanding proposed theories. The theory at a time that Heraclitus proposed was that the principal of change was the only basic law governing the universe and that everything changes. Therefore, the role of time in the universe was being investigated.

The inclusion of African perspectives in the physics curriculum is purported to build self-esteem to an African child, seeing her ancestors having contributed to the body of knowledge. The underlying message is that physics is for everyone not for the select few.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Theoretical and Computational Physics / 336

Balance in Quantum Dynamical Systems

Author: Rocco Duvenhage[1]

Co-author: Mathys Snyman [2]

[1] *University of Pretoria*

[2] *Akademia*

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Using a study of the connection between entanglement and quantum detailed balance as motivation, we introduce the concept of balance between two quantum dynamical systems. The definition of a quantum dynamical system used is a von Neumann algebra with a faithful normal state, and a state preserving unital completely positive map. It is showed how balance can be used to find relaxed versions of properties related to equilibrium, such as quantum detailed balance conditions, and that it provides a mathematical framework within which the question of transfer of properties between systems in balance can be investigated. Promising recent research with regard to the latter using Wasserstein distances is briefly discussed.
The role of functional analysis and specifically Tomita-Takesaki theory in establishing this framework is also discussed.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Astrophysics & Space Science / 337

Compton polarization signatures in gamma-ray burst models

Author: Pieter Van der Merwe[1]

Co-author: Markus Bottcher [2]

[1] *North-west University, Center for Space Research*

[2] *University of North West*

Corresponding Author: pietervdmerwejnr@gmail.com

Since the first detection of gamma-ray bursts (GRBs) in 1967, GRBs have been an active subject of study with many questions still left unanswered. Though the physics of GRB afterglows is relatively simple and more well known, there is still much discussion regarding that of the prompt emission phase of GRBs. Several models, including synchrotron models with both ordered and random magnetic fields, synchrotron self-Compton models as well as Compton-drag models and photospheric models have been proposed in order to explain the Band-like spectra of GRB pormpt emissions. Seeing as both synchrotron radiation and anisotropic Comptonization (as expected in both photospheric and Compton-drag models) may lead to X-ray polarization, it is inevitable that polarization predictions from the various proposed models should be used in conjunction with X-ray polarization measurements by POLAR and possibly the future COSI missions in order to investigate the emission mechanisms of GRBs. In light of this, we develop a Monte Carlo polarization code, heavily inspired by the MAPPIEs code, to estimate Compton polarization signatures from various GRB models in order to constrain and hopefully discriminate between the available models.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 1 / 338

Investigation of reduced graphene oxide as an alternative carbonaceous material for lithium ion batteries: A density functional theory study

Author: Thokozane Mxolisi Mlotshwa[1]

Co-authors: Lordwell Jhamba [1]; Joseph Kirui [1]; Eric Maluta [1]

[1] *University of Venda*

Corresponding Author: thokozanimxolisi@gmail.com

Producing electrical energy from fossil fuels proves to be a growing concern and requires alternatives for it to be sustainable. The electrical generation capacity is still not enough. Renewable energy (RE) generation faces an uncertain future as most of its generation processes require favorable conditions, the sun must shine or the wind blows. One way to ensure continuous supply of renewable energy is to have a storage device to store excess energy produced during those sunny and windy days. Available storage devices however suffer from low energy densities, very expensive and short lifespan. The full-scale development of lithium-ion batteries is largely limited by the energy density. A lot of research is carried out to address the low energy density in recent years but it is still low to meet the fast pace development of materials and machinery. The current study uses density functional theory for reduced graphene oxide (RGO) analyses to use in lithium ion batteries. Our results

suggest that RGO possesses excellent properties for use in lithium ion batteries for improved energy storage.
Keywords: Renewable energy, reduced graphene oxide, Lithium-ion, energy storage

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Poster Session 2 / **339**

Design of a PV power system for grid-connected Facilities energy retrofitting: A case study of 15 SAI Battalion, Limpopo Province in South Africa

Author: Sophie Mulaudzi[1]

Co-authors: DAVID TINARWO [2]; vhutshilo 1st mountaineer nekhubvi [2]; Nnditshedzeni Eric Maluta [1]; Donald Mashaba [1]

[1] *University of Venda*

[2] *UNIVERSITY OF VENDA*

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With global threats to energy security, the need for diverse energy sources is becoming increasingly important. Nations, communities, and individual energy consumers need more locally available and accessible renewable energy sources to form part of diverse energy sources mix for a sustainable supply of their local energy demand. A country like South Africa, overwhelmed with demand against dwindling power supply, which has led to the implementation of load shedding, can only put its hopes to a decentralised distributed generation where individual consumers generate power onsite to cover their needs partially or wholly. Besides serving local consumers with an uninterrupted energy supply, distributed local renewable energy generation contributes to easing pressure on the electricity grid and reducing greenhouse gas emissions. This study comprehensively analyses the calculation of an optimally designed grid-connected photovoltaic (PV) system's energy output. Monthly solar radiation data was assessed, and average sunshine hours were generated to design the 15 SAI Battalion sick bay electric power supply connected to the grid. Individual rooms appliances inventory with electric parameters and time of use data was done for all rooms for energy use audit. Due to the high total load power and financial constraints, the power systems were designed to cover part of the load of the building. PVSyst and HOMER software were used to design and optimise the system dispatch. The analysis of this study highlights the potential benefits of grid-connected PV systems, underlining their role in improving local energy supplies and relieving the electricity grid's burden.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Applied Physics / **340**

Topic: Conversion of biomass into carbonaceous material: Making synthetic graphite

Authors: Pfano Nemakonde[1]; Fhulufhelo Nemangwele [1]

Co-authors: Thokozane Mlotshwa [1]; Lordwell Jhamba [1]

[1] *University of Venda*

Graphite is the most valuable material with many applications such as lithium-ion batteries as anode material. The increase in demand for storage devices prompted researchers to consider other possible, low cost and commercially viable alternatives to meet the demand. The synthesis and application of biomass as carbon have drawn attention due to the host of biomass available for conversion, sustainability and cost effective. The current work focuses on converting biomass wastes into synthetic graphite. Heat is used to process biomass into desired carbon product. The FTIR and UV-vis spectra suggests successful conversion of biomass into carbon. The results show that the obtained graphite-like crystallite-based nanomaterials with tunable dimensions and morphologies has remarkable features, such as high water solubility

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

Hons

Physics of Condensed Matter and Materials Track 1 / 341

Development of 2D/3D stable tin-based halide perovskite solar cell

Author: Mmantsae Diale[1]

[1] *University of Pretoria*

Corresponding Author: mmantsae.diale@up.ac.za

The successful use of Sn-based material as light absorber in Schottky barrier solar cell with a PCE efficiency of 0.9%, encouraged researchers to pursue the material as a possible replacement of lead for stability of perovskites. This led to the development of 2D/3D Sn-based perovskites as prospective future candidates for stable HaP solar cell, where the photo conversion efficiency (PCE) has steadily increased to 14.81%. However, the fast and easy oxidation of Snˆ(2+) to Snˆ(4+) in the system contributes to poor stability and low PCE of Sn-based perovskite solar cells. In this work, SnF2 was gradually introduced in the FASnI3 perovskite precursor solution alongside N-N'-diphenyl-P-phenylenediamine (DPP-DTT) antioxidant as a co- additive, and their effect on the performance and stability of the perovskite film studied. The results show improved stability from less than an hour with SnF2 alone to more than 1300 hours with DPP-DTT. A 3D planar inverted FTO/PEDOT:PSS/FASnI3/PCBM:P3HT/Ag structure was fabricated. The results show improved stability from less than an hour with SnF2 alone to more than 1300 hours with DPP-DTT.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Applied Physics / **342**

The work of Physics to mitigate greenhouse gases to address climate change.

Author: Mmantsae Diale[1]

[1] *University of Pretoria*

Corresponding Author: mmantsae.diale@up.ac.za

The earth has experienced extreme weather changes due to irresponsible human activities done ignorantly by passengers. The passengers are contaminating the atmosphere with greenhouse gases, polluting the environment with non-degradable materials, not considered renewable and green. This paper presents the status quo of the world methods to produce clean and green energy, with better methods due to physics innovations. These includes using physics in waste recycling, synthesis of new materials and devices, and green electronics, collection of electricity from sun, wind and hydroelectric energy.Using of solar panels instead of diesel generators during load shedding, consciously cleaning the environment by using packaging that is biodegradable and calculating the carbon footprint.

Apply to be considered for a student ; award (Yes / No)?:

no

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Consent on use of personal information: Abstract Submission:

Poster Session 1 / **343**

Chemical Trends in defect stability and electronic properties of 3d transition metal doped WS2

Author: Brian Nyandoro[1]

Co-author: Evans M Benecha [1]

[1] *Unisa*

Corresponding Author: brinyandoro@gmail.com

Dilute magnetic semiconductors (DMSs) offers an alternative pathway towards achieving electronic hybrid devices capable of combining the three critical functionalities of logic, communication and data storage, within a single IC chip. Such DMS hybrid devices can use both voltage and light to simultaneously manipulate both the charge and spin of an electron promising more affordable, compact and faster multifunctional chips with lower power consumption. Two dimensional (2D) transition metal dichalcogenides (TMDCs) have promising magnetic properties suitable for DMS applications due to their superior spin relaxation times and diffusion lengths. In contrast to graphene, TMDCS exhibit a tuneable bandgap and stronger spin-orbit coupling which are a prerequisite for spin logic and non-volatile data storage. However, TMDCs are not intrinsically magnetic, hence, it is important to engineer magnetism in them in order to realize their potential as DMS materials.

In this work, we investigate the energetic stability and electronic properties of 3d transition metal defects in single layer WS2 at different lattice locations, using Density Functional theory electronic structure calculations. We find that the chemical stability of a transition metals in WS2 is strongly dependent on the doping lattice site, and its ‘d’ character across the 3d series.
Specifically, from Sc to Co, the substitutional site is found to be energetically more favorable with

lower formation energies in comparison to the adatomic and interstitial doping. However, from Ni to Zn, the energetic stability shifts towards the adatomic doping location, with the substitutional site becoming highly unfavourable. Even though intrinsic monolayer WS2 has a direct bandgap, we find that doping does not always preserve the direct bandgap. Furthermore, incorporating 3d transition metal atoms into its lattice introduces defect energy levels within the bandgap, with the band gap of doped WS2 increasing by 1.2 eV from Sc to Mn, while narrowing down by 1.3 eV from Mn to Zn. Furthermore, we find that increasing the dopant concentration lowers the formation energy in WS2, favouring clustering. These results present important implications to the understanding of the properties of transition metal dopants in WS2, as well as in other dilute magnetic semiconductors where the effect of aggregation of dopants has generally been neglected.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Theoretical and Computational Physics / **344**

Continuous Monitoring and Feedback Control of a quantum harmonic oscillator

Author: Thomas Konrad[1]

Co-author: Amy Rouillard [2]

[1] *UKZN*

[2] *University of KwaZulu-Natal*

Corresponding Author: konradt@ukzn.ac.za

I review quantum state monitoring and measurement-based feedback control at the example of a particle in a harmonic potential [1]. Feedback can be employed to effectively modify the Hamiltonian, dissipate energy and transfer the system into the ground state while simultaneously compensating the noise introduced by the continuous measurement.

[1] A.Rouillard, A. Reddy, H. Bassa, S. Maharaj, L. Diosi and T. Konrad
Measurement-based Feedback Control of a Quantum System in a Harmonic Potential,
preprint: arXiv:2212.12292,(2022) link: [2212.12292] Measurement-based Feedback Control of a Quantum System in a Harmonic Potential

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Astrophysics & Space Science / **345**

Application of Data-Driven Deep Learning Hybrid Models for Forecasting of Semidiurnal and Diurnal Tides Measured by a SuperDARN HF Radar

Authors: Nkanyiso Mbatha[1]; Venkataraman Sivakumar[2]

[1] *University of Zululand*

[2] *University of KwaZulu Natal*

Corresponding Author: nkanyisombatha5@gmail.com

Semidiurnal and diurnal tides are known to have a significant impact upon the momentum balance in the mesosphere-lower thermosphere (MLT) region, and on the distribution of atmospheric constituents. In general, tidal structures in the middle atmosphere are exceptionally complex, and thus their successful modelling
requires consideration of a wide range of atmospheric phenomena, such as radiational, chemical, and dynamical processes. The recent developments in the field of machine learning and deep learning data-driven time series forecasting models have opened an opportunity to forecast complex time series such as atmospheric tide. Therefore, the main aim of this study is to extract and analyze tidal wave information from Kerguelen SuperDARN High-Frequency (HF) radar zonal and meridional wind components using Short-Time Fourier Transform (STFT), and to forecast the tidal waves amplitude time series using hybrid deep learning neural
networks models. The model used here is the long short-term memory networks (LSTM) recurrent neural networks (RNNs), a robust data-driven hybrid time series-forecasting model which is based on signal decomposition techniques such as Ensemble Empirical Mode Decomposition (EEMD), and Empirical Wavelet Transforms (EWT). To compare the modelled data to the ground truth, the tidal wave data is divided into 80% training time series and 20% testing time series. In general, the results highlight that the EWT-LSTM model outperforms the other models in terms of accuracy and error reduction in the forecasting of both semidiurnal and diurnal tides. Signal decomposition seems to enhance the performance of the model when compared to the use of the LSTM model as a standalone.

Keywords: Tides, LSTM, forecasting, Middle Atmosphere, neural networks
Emails: MbathaN@unizulu.ac.za , Venkataramans@ukzn.ac.za

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / **346**

Microstructural characterization of low elastic modulus β-Ti alloy fabricated by arc melting process

Authors: Mandy Madigoe[1]; N Nyakane[None]; R Modiba[None]

[1] *CSIR*

Corresponding Author: mseerane@csir.co.za

Development of low elastic modulus β-Ti alloys for implant application has grown significantly in recent years. In this work, alloy Ti-28.3Nb-13.8Ta-6.9Zr was produced by button arc melting (BAM). Pure metal powders of Ti, Nb, Ta and Zr were pre-mixed and prepared as feedstock powder to the Copper-Hearth BAM. The alloy was manufactured, and heat treated (HT - solution treated + aged). The samples were analyzed for microstructure using the following techniques – OM, ImageJ, SEM-EDX, XRD and EBSD. The alloy showed a dominant β-phase microstructure in a dendritic morphology in both the as-cast and heat treated condition. The microstructure was characteristic of Ti-Nb-Ta-Zr (TNTZ) alloys. The EBSD results will be presented.

Key words: Low modulus, β-Ti, implant, arc melting, heat treated, microstructure.

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 1 / **347**

Gas sensing properties of rare-earth substituted MgFe2O4 ferrite nanoparticles

Authors: Prince Mkwae[1]; Nolitha Ngubelanga[2]; Ceboliyazakha Ndlangamandla[3]

[1] *University of KwaZulu-Natal*

[2] *University of Fort Hare*

[3] *University of Zululand*

Corresponding Author: mkwaeps@yahoo.com

MgCexFe 2-xO4 ($0 \leq x \leq 0.4$) nanoparticles have been produced by the glycol-thermal technique and characterized by X-ray diffraction, electron microscopy, X-ray photoelectron spectroscopy, Mössbauer spectroscopy, and gas sensing analyses. The X-ray diffraction results indicated that a pure cubic spinel phase was formed for samples having a low concentration of Ce, but the high Ce doping ($x < 0.2$) of magnesium ferrite resulted in the formation of secondary phases. The crystallite size of the compounds ranged from 2.2 nm to 15.3 nm. The 57Fe Mössbauer spectra showed the transformation from an ordered to a paramagnetic spin state with an increase in Ce concentration. Gas sensors fabricated from the spinel ferrites were tested towards various organic compound vapours (acetone, methanol, p-xylene, ethylbenzene, toluene, and benzene) at an operating temperature of 225 ℃. The MgCe0.2 Fe1.8O4 nano ferrite proved to possess quality sensor characteristics of high sensitivity and selectivity to acetone vapour, with a response of over 500@100 ppm concentration as well as reproducibility, reversibility, and stability of over 120 days.

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Poster Session 2 / **348**

Simulating the position sensitivity of a large-volume segmented germanium clover detector

Authors: Sive Noncolela[1]; Elena Lawrie[2]; Nico Orce[3]; Sifiso Senzo Ntshangase[4]

[1] *UWC*

[2] *iThemba LABS*

[3] *University of the Western Cape*

[4] *University of Zululand*

Corresponding Author: prosive@yahoo.com

The iThemba LABS segmented clover detector (TIGRESS type) comprises four HPGe crystals, each one segmented eight-fold. Such new generation Ge detectors are able to perform γ-ray tracking but are more complex to work with. In order to properly maximise the use of this detector a method to locate gamma-ray interaction points within the detector was developed. The gamma ray interaction points were reconstructed at different radial and azimuthal positions around the detector volume. Multi Geometry Simulation (MGS) and Advanced Detector Libraries (ADL) were used to simulate the detector response at different positions. The response of an HPGe detector was also experimentally determined for certain positions around the detector to a particular energy deposited at a well-defined (x,y,z) location. This was done by using a scanning table where gamma rays were collimated to target a particular interaction point on the detector and digitized pulses were recorded for those points. An average of all characteristic waveforms was performed for each point to minimize noise fluctuations. The experimental waveforms were compared to the simulated ones where experimental corrections such as crosstalk were also performed. Corrections for the response function of the preamplifier were also incorporated in the signal output.

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Photonics / **349**

Modal Characterization of a Few-Mode Fiber based on a Wavelength and Polarization Entangled Photon Source

Authors: M Youssef[1]; S Colombel[1]; D Sengupta[1]; C Tremblay[1]; B Ung[1]

[1] *Electrical Engineering Department, École de Technologie Supérieure (ETS)*

Corresponding Author: mostafa-ahmed-fouad.youssef.1@ens.etsmtl.ca

High-dimensional quantum states, known as qudits, have the potential to enhance the performance of quantum information systems. One promising approach for devising and delivering qudits is to exploit the multiple modes of a few-mode fiber (FMF) as the carriers of the quantum states. In this work, we show the excitation, transmission and detection of wavelength-entangled photons in a few-mode fiber. We show that the distinctive peaks in the time-correlation histograms can be ascribed to different propagation modes of the fiber. Furthermore, we measure the polarization dependence of the fiber-based source of entangled photons (in the C+L telecom bands), and show that although the state-of-polarization (SOP) of a given photon (e.g., the C photon) is completely random, its twin photon (e.g., L photon) retains a good level of polarization entanglement. This work is part of ongoing research in high-dimensional quantum key distribution schemes based on FMF.

Apply to be considered for a student ; award (Yes / No)?:

yes

Level for award;(Hons, MSc, PhD, N/A)?:

PhD

Plenary 3 / **350**

Who needs non-hermitian quantum mechanics?

Author: Hendrik Geyer[1]

[1] *Stellenbosch University*

Corresponding Author: hbg@sun.ac.za

I'll introduce some basic quantum mechanics and simple models from nuclear physics to show how and why non-hermitian operators enter into quantum mechanics in the first place. This will be followed by discussing how one can construct a fully self-consistent non-hermitian quantum mechanical framework and how this relates to so-called PT-symmetric quantum mechanics. I'll conclude by discussing how this work has impacted recent work in optics and other fields of physics.

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Plenary 4 / **351**

What is like to be a woman in Physics: Life-Experiences, Success, and Challenges

Author: Gugu Mhlongo[1]

[1] *CSIR/UFS*

Corresponding Author: gmhlongo@csir.co.za

To be uploaded.

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Plenary 1 / **352**

Unifications in particle physics: from coupling crossing to asymptotic unification

Author: Aldo Deandrea[1]

[1] *IPNL*

Corresponding Author: deandrea@ipnl.in2p3.fr

The structure of the Standard Model of particle physics inspired the idea that, at high energy, a simple unified description is possible in terms of only one unified gauge coupling. Various approaches, with different gauge groups describing the unified theory, were proposed, but realistic models are typically non-minimal. After introducing the historical path that led to these theories I will discuss a new possibility where the gauge couplings evolve asymptotically towards the same fixed point at high energy.

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Photonics / **353**

From quantum quirks to microscopic wonders: journey into the future of imaging with entangled photons!

Author: Hugo Defienne[1]

[1] *Institute of Nanosciences of Paris at Sorbonne University*

Corresponding Author: hugo.defienne@insp.upmc.fr

Quantum physics may be at the origin of tomorrow's microscopes - let's understand how it works!

Quantum imaging harnesses quantum properties of light to go beyond the limits of classical imaging. In this respect, entangled photons sources are very promising. They have been proposed and used to achieve super-resolution and sub-shot-noise imaging, and to create new imaging approaches such as ghost imaging, quantum illumination and quantum holography. In this non-specialist presentation, I will review some recent imaging techniques based on entangled photon pairs that have been developed in recent years. I will discuss some fundamental aspects of these approaches, including the critical role of entanglement, but I will also insist on their application potential for microscopy.

Apply to be considered for a student ; award (Yes / No)?:

No

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Theoretical and Computational Physics / **354**

Theoretical and Computational Division meeting

Corresponding Author: alanc76@gmail.com

The theoretical and computational division meeting

Astrophysics & Space Science / **355**

Division Meeting

Plenary 7 / 356

Exact Quantitative Analysis of Low-Dimensional Quantum Structures using Alkali-Metal based Molecular-ion SIMS: Perspectives and Challenges

Author: Purushottam Chakraborty[None]

Continuous progress in the understanding of fundamental and instrumental aspects of Secondary Ion Mass Spectrometry (SIMS) has made this technique extremely powerful for the analysis of materials. Secondary ion-emission is a complex phenomenon and amongst various mechanisms, the 'electron-tunnelling model' based on the survival probability of an escaping ion above the surface is the widely accepted notion in the understanding of ionization probability for positive and negative ions. As the secondary-ion intensity of a particular element strongly depends on the ionization efficiency of a sputtered atom or molecule, instantaneous local chemistry of the sample surface plays a significant role in the secondary-ion emission. This is the so-called "Matrix Effect", which makes the SIMS technique challenging for quantification in spite of its highest detection sensitivity (<ppb) and exceptional depth-resolution (<1nm). Therefore, the compensation of "matrix effect" is required. If alkali-metals such as Li, Rb, K, Na, Cs, ...etc. (referred to as 'A') are present in the neighbourhood of the probing element (M) on a sample-surface, a quasi-molecular (MA) + ion can be formed by the attachment of this alkali-ion with a sputtered atom (M 0) in the close proximity of sample surface. Such phenomenon can occur if an alkali-ion beam is chosen as the impinging ion-beam for sputtering. The (MA) + molecular-ions that are formed in the SIMS process have strong correlation with the atomic polarizability of the element M. As the emission process for M 0 is decoupled from the MA + ion formation process, the 'matrix effect' drastically decreases. This is
very similar to the ion formation in "secondary neutral mass spectrometry" (SNMS). Although the detection of (MA) + molecular ions has found its applicability in materials quantification without calibration standards, it generally suffers from a low useful yield. In such case, the detection of (MA) 2 + molecular-ions offers a better sensitivity (by orders of magnitude), as the yields of (MA) 2 + molecular-ions have been found to be much higher compared to that of (MA) + molecular-ions.

Monitoring of molecular-ions is often employed in standard SIMS experiments to improve the detection of sputtered ion-species which show poor dynamic ranges or are affected by mass interference. For example, while making SIMS analysis of GaAs, carbon as an impurity-element is detected by monitoring (AsC) + molecular-ions instead of C - ions, because the latter has a high background arising from residual-gas species in the analysis chamber. Cs is highly preferred for MCs +
or MCs 2 + molecular-ions in SIMS because of the strongest reactivity and electropositive nature of caesium.

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Consent on use of personal information: Abstract Submission:

Yes, I ACCEPT

Poster Session 2 / 357

Opto-functional characteristics of merit in graphene oxide and reduced graphene oxide from synthetic graphite feedstock for potential incorporation in thin film organic solar cells

Author: Marry Thekhwe[1]

Co-authors: Lordwell Jhamba [1]; Fhulufhelo Nemangwele [1]; Thokozane Mxolisi Mlotshwa [1]

[1] *University of Venda*

Corresponding Author: thekhwemarry@gmail.com

This work derives from the problematic low performance of organic solar cells (OSCs) and attempts to make a contribution to its improvement through an empirical exploration of the potential of graphene derivatives, graphene oxide (GO) and reduced graphene oxide (rGO), for incorporation in OSCs. Along this, GO and rGO were synthesized from the primary feedstock, synthetic graphite (SG). GO was synthesized using the modified Hummers' method, while rGO was synthesized using the modified Tour method. The intrinsic properties of these graphene derivatives were searched for through characterization technique engagements due to Fourier Transform Infrared (FTIR) spectroscopy and Ultraviolet (UV-vis) spectrophotometry, followed by analysis. GO and rGO have been found to be having properties (for example, improved electrical conductivity and light absorbance) that favour their incorporation in organic solar cells, for performance enhancement of the cells.

Apply to be considered for a student ; award (Yes / No)?:

Yes

Level for award;(Hons, MSc, PhD, N/A)?:

Hons

Applied Physics / **358**

Applied Physics Division Meeting

Corresponding Author: matthewsa@ukzn.ac.za

Plenary 2 / **359**

Leveraging MeerKAT to train the next generation of South African astrophysicists

Author: Kenda Knowles[None]

When South Africa applied to host the Square Kilometre Array (SKA) project in the mid-2000s, a decision was made that, irrespective of the outcome of the bid, the country should build and host a premier radio telescope of their own. Thus the MeerKAT was born and has become a world-renowned instrument during its first five years of operation, producing ground-breaking science in a wide range of research areas. With South Africa to host the mid-frequency component of the SKA, MeerKAT plays a critical role in developing local human capital who will use the major radio observatories of the future. In this talk I will discuss some of the science being done with MeerKAT and how these projects are helping to train the next generation of African astronomers.

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Consent on use of personal information: Abstract Submission:

Yes, I ACCEPT

Plenary 5 / **360**

Topological Materials with Intriguing Magnetic Textures.

Author: Jeffery Lynn[None]

The topic of magnetoelectronic properties of topological materials is of high interest from both the fundamental physics and applications viewpoints. Our focus is on systems that exhibit long range magnetic order, investigated via neutron scattering, and how that order tailors the electronic properties. One interesting example is provided by the tetragonal CeAlGe material, where the strong coupling of the magnetic order with the Fermi topology allows a singular angular magnetoresistance to emerge. For YMn 6 Sn 6 , on the other hand, the magnetic structures in the appropriate temperature and magnetic field regime are incommensurate in nature with concomitant strong spin fluctuations that give rise to a large topological Hall effect. This topological Hall effect has a completely new origin based on thermal fluctuations, which naturally develop at elevated temperatures. Both of these examples beautifully demonstrate the synergy between transport measurements, neutron scattering determinations, and theoretical calculations to understand the properties. Finally, we present recent work on systems where the large moment magnetism of the isotropic spin-only Eu 2+ rare earth ions provide platforms for field-induced topological Hall regimes, or coupled charge and spin orders, or a system with an exceptionally high electron mobility that allows an intrinsic spin Moiré superlattice to emerge

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

Consent on use of personal information: Abstract Submission:

Yes, I ACCEPT

Plenary 8 / **361**

Physics in the financial markets

Author: Anthonie Kotze[None]

What can a physicist do in the financial markets? I will discuss the plenty of opportunities to practise physics, mathematics and statistics and that one can survive and thrive. Physicists in the financial markets are named quants (quantitative analysts), rocket scientists and financial engineers.
An applied mathematician and two economists reshaped the financial markets in 1973. Two received the Nobel prize for economics in 1997. I will discuss the Black-Scholes-Merton equation and why it is so significant and necessary in our modern age of trading and hedging foreign exchange, equities and interest rates. Instruments like swaps, options, futures and credit default swaps are called derivatives

and are traded daily at banks and stock exchanges around the globe. Global trade and investments cannot blossom without these instruments, and we will show you why.

Apply to be considered for a student ; award (Yes / No)?:

N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

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Yes, I ACCEPT

Plenary 6 / **362**

Ion beam Modification and Characterization of Materials Two examples from measurements at the rib facility ISOLDE at CERN

Author: Krish Bharuth-Ram[None]

Two initiatives drive our current research in ion beam modification of materials: a) Search for spintronic oxide and nitride semiconductors, i.e. semiconductors doped with very low concentrations (≤ 5 at. %) TM ions, the so-called dilute magnetic semiconductors (DMS), which if realized would have room temperature ferromagnetism (RTFM) coexisting with the charge carrier semiconducting functioning of the system, and b) Determination of the lattice occupancy of heavy ions implanted in diamond. Studies (a) were conducted in 57 Fe-emission Mössbauer Spectroscopy (eMS) measurements following implantation of precursor radioactive 57 Mn * ions into host substrates at the online radioactive ion beam facility ISOLDE at CERN. EMS measurements on ZnO show strong magnetic sextets in the spectrum but the magnetic field shows no dependence on temperature, hence ruling out ferromagnetic behaviour. Further measurements on ZnO pre-implanted with C, Ar, Fe and Co ions show similar results. In studies (b), over the years (since 1993) we have conducted Emission Channeling (EC) measurements on a range of radioactive (Li, P, Fe, Cu, Ce, Gd, Er) ions implanted in diamond. The lattice occupancy of the probe ions is extracted from channeling effects on the emitted decay products of the probe nuclei by the positively charged atomic rows of the crystal lattice. These lead to anisotropic yields of the ⍰-particles, conversion electrons or ⍰-
particles emitted by the nuclear probes with respect to the major lattice directions of the host. Sample results will be presented of eMS measurements on ZnO and of EC measurements on Er and TM ions implanted in diamond.

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N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

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Applied Physics / **363**

Applied Physics Division Meeting

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Photonics / **364**

Photonics Division Meeting

Corresponding Author: pietern@sun.ac.za

Nuclear, Particle and Radiation Physics / **365**

Division Meeting: Nuclear, Particle and Radiation Physics

Corresponding Author: edward.khomotso.nkadimeng@cern.ch

Physics for Development, Education and Outreach / **366**

Physics in Business: survival in the jungle

Author: Irvy (Igle) Gledhill[1]

[1] *U. Witwatersrand*

Corresponding Author: igle.gledhill@wits.ac.za

In industry and in large companies, physicists face a variety of challenges. Some are minor, like the Einstein stereotype, and some are significant, for example adapting to a hierarchy. In this talk we'll take a look at what drives a company and how the drivers affect the work of the physicist. We'll talk about the context of research and innovation in the private sector and explore some of the contrasts between entrepreneurial tech startups, private companies, and science councils. There will be a quick overview of the role of project management, types of leadership, and change-making. That will lead to the links between the physicist and people in the legal, finance, procurement, and human resources arms of the company. Into this background fabric, I will weave some of the challenges and exhilaration that a physicist encounters in the company space and industrial time-scales, and identify a few of the tools that might be found useful in navigating the business jungle.

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N/A

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N/A

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Poster Session 2 / **367**

Signatures of possible trinni event during quiet geomagnetic conditions

Author: Zolile Mtumela[1]

[1] *University of KwaZulu-Natal*

Corresponding Author: 208516464@ukzn.ac.za

A study of a single event to investigate signatures of possible trinnis event during quiet geomagnetic conditions. One of the signatures of trinni event is the high-speed flows, which were interpreted to be associated with the release of energy from a rapid reconfiguration of tail magnetic field lines due to magnetic reconnection. This type of event is known to be “trinni” event, using the SuperDARN data from the northern and southern hemisphere. Then objective of this case study is to identify signatures of trinni event, using the SuperDARN data from the northern and southern hemisphere. The study presents the situation where the y-component of the interplanetary magnetic field (IMF) dominates over the z-component, the directions of both the high speed flows and the underlying convection pattern depend on the direction of the IMF By-component. The assumption both non-substorm interval and quiet condition are justified by the magnetometer, GOES satellite data, geomagnetic indices, and the observations are discussed in relation to magnetic reconnection in the magnetotail.

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N/A

Level for award;(Hons, MSc, PhD, N/A)?:

N/A

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Astrophysics & Space Science / 368

Star-forming galaxies and radio-active galactic nuclei in the faint radio sky

Author: Getrude Thando Mothogoane[1]

Co-authors: Sthabile Kolwa, ; Soebur Razzaque

[1] *University of Johannesburg*

Corresponding Author: ramodubjane@gmail.com

Understanding the complex relationship between nuclear activity, star formation, and galaxy growth is crucial for disentangling the mechanisms driving galaxy evolution. This project investigates how nuclear activity regulates star formation and galaxy growth at higher redshifts (z > 1). We specifically explore the correlations between black hole accretion rate (BHAR), star formation rate (SFR), and stellar mass (M *) in both star-forming galaxies (SFGs) and host galaxies of radio active galactic nuclei (AGN). Utilizing MeerKAT International GHz Tiered Extragalactic Exploration (MIGHTEE) Early Science data from the COSMOS field, along with multiwavelength ancillary data, we aim to constrain the physical properties of SFGs and radio AGN host galaxies within a redshift range of 0 ⊠ z ⊠ 6. By analyzing the data, we determine the SFR, M * , and dust luminosity (L dust) for these sources using spectral energy distribution (SED) fitting techniques. To achieve this, we compare the results obtained from four SED fitting codes: MAGPHYS (da Cunha et al. 2008), CIGALE (Noll et al. 2009), AGNfitter (Calistro et al. 2016), and MrMoose (Drouart et al. 2018). The comparison is made against physical properties derived from independent measurements. The goal is to select the SED fitting code that yields physically feasible results and performs well for very faint radio sources.

By utilizing MeerKAT observations, multiwavelength data, and SED fitting techniques, this project aims to analyze the physical properties and investigate the correlations between nuclear activity, star formation, and
galaxy growth. The findings of this study will contribute to our understanding of the underlying physical mechanisms driving star formation and quenching across cosmic time.

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Astrophysics & Space Science / 369

Division Meeting

Physics of Condensed Matter and Materials Track 1 / 370

Division Meeting: Condensed Matter and Materials Science

Corresponding Author: rudolph.erasmus@wits.ac.za

Physics for Development, Education and Outreach / 371

Nanoscience innovations: On the trapping of cold neutrons in nano-scaled Fabry-Perot resonating cavities & neutron lifetime considerations

Author: Malik Maaza[None]

Relatively to the atomic constituents' counterparts, the neutron is singular as it is sensitiveto the four fundamental interactions: strong, weak, electromagnetic, and gravitational. This multi-sensitivity makes neutron wave-matter optics a particularly versatile tool for testing quantum mechanics specifically and fundamental physics concepts in general.The lifetime of a free neutron defined via its beta-decay ⟨τn⟩ is of a pivotal importance within the standard model cosmology. Indeed, the precision on the neutron lifetime is paramount as it regulates the precision of the 1st element of the Cabibbo–Kobayashi–Maskawa matrix, central to the standard model. The two major methods used to measure ⟨τn⟩ while trapping free neutrons, namely, the beam and the bottle methods give different neutron lifetime values; ⟨τn⟩Beam ~ 888.0 ± 2.0 s , that obtained by the bottle technique is smaller; of about ⟨τn⟩Bottle ~ 879.4 ± 0.6 s. In addition of the persistent difference of ~10 s persists for years, even if the two methods have been modified to enhance the experimental accuracy. This latter was shown to be enhanced if one could trap cold neutrons in nanostructured Fabry-Perot resonators. The de Broglie wave-particle duality coupled to the Fermi total reflection phenomenon in addition to the tunneling trapping of cold neutrons in such nano-resonating cavities, allow trapping times with a precision governed by the Heisenberg uncertainty of 10 -12 s

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N/A

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Physics for Development, Education and Outreach / **372**

Intellectual Property, Innovation Management and the Role of NIPMO in Innovation Support in South Africa

Author: Thabang Jase[None]

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N/A

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Physics for Development, Education and Outreach / **373**

Innovation and Technology Transfer

Author: Pragasen Mudali[None]

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Test Session / **374**

Test Abstract 29 September 2023

Author: Tebogo Mokhine[1]

[1] *SAIP*

Corresponding Author: tebogo.mokhine@saip.org.za

For presentation purposes...

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N/A

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375

Developing a Nuclear Orientation Thermometer for the UCT Dilution Refrigerator

Author: Yanga Ntolosi[1]

Co-authors: Stephen Peterson [2]; Mark Blumenthal [2]; Dominique Gouveia

[1] *NMISA*

[2] *University of Cape Town*

Corresponding Author: syntolosi@gmail.com

A significant challenge in low temperature thermometry is the accurate measurement of temperatures below 1 k. Nuclear Orientation (NO) is a non-electronic technique to measure ultra-low temperature accurately as opposed to traditional resistive thermometers. The NO method relies on the measurement of the alignment of the nuclear spin in a radioactive nucleus, where the temperature can be derived from the Boltzmann distribution.
The aim is to develop a NO thermometry system using the recently procured gamma-ray anisotropy thermometer (60CoCo(hcp)) source for use in the University of Cape Town Department of Physics dilution refrigerator. The UCT dilution refrigerator is able to achieve these ultra-low temperatures (down to 8 mK) by taking advantage of the properties of both 3He and 4He gas.
The 60CoCo(hcp) radiation source, irradiated using the SAFARI-1 research reactor at NECSA, is incorporated into the dilution fridge by thermally mounting it onto the plate in which the mixing chamber is positioned. The data acquisition system, a Sodium Iodide (NaI) scintillation detector, is placed in line with the source allowing it to detect the radiation as accurately as possible. The ratio of the detected radiation at various temperatures provides the measurement of nuclear spin alignment and thus the absolute temperature of the system. The preliminary measurements are promising, but more work needs to be done in order to develop a fully-functioning NO temperature measurement system.

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Yes

Level for award;(Hons, MSc, PhD, N/A)?:

MSc

Photonics / **376**

Test

Author: Tebogo Mokhine[1]

[1] *SAIP*

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