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Book of Abstracts

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Landau criteria for superfluidity for a mixture of Boson & Fermions

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The phenomena of superfluidity was first observed in liquid Helium by Kapitza in 1938. Superfluidity is the friction less flow of atoms or molecules without dissipation at very low temperatures. There is a critical temperature below which the assembly of interacting particles , bosons , or fermions , or a mixture of bosons and fermions becomes superfluid leading to a phase transition from the so -called normal phase to superfluid phase. Thus there was a need to explain why a mass of atoms could be transported without friction and dissipation in the superfluid phase . Such a criteria was proposed by Landau according which the mass transport can take place without dissipation for some critical velocity. To calculate the critical velocity, first the quasi-particle energy expression for an interacting assembly of bosons and fermions is obtained by diagonalizing the model Hamiltonian of an assembly of interacting bosons and fermions . At the minimum value of the momentum in the superfluid state, the critical velocity is calculated .
The assembly sustain superfluidity if the velocity of flow is less than the Landau Critical velocity. The mixtures studied are Li 6 (fermion)+Li 7(boson); Rb 87 (boson)+K40(fermion)

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COST OF CLOUD COMPTUTING ON RECORD MAINTENANCE IN NYANDARUA INSTITUTE OF SCIENCE AND TECHNOLOGY, NYANDARUA COUNTY, KENYA

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ABSTRACT
The study sought to establish the effect of the cost of cloud computing on record maintenance in the Nyandarua Institute of Science and Technology. The specific objective of the study was to establish the effect of the cost of cloud computing on record maintenance in the Nyandarua Institute of Science and Technology. A quantitative and qualitative research design was used in this study.The population contained 125 respondents. The relationship between the variables was established through correlation analysis. On whether loss of records can have a major impact on the institutions in terms of cost of recovery it was established from the findings that 65% of the respondents agreed, 25% strongly agreed, 5% strongly disagreed and 4% disagreed while only 1% was neutral. Finally, the respondents were asked to state whether record maintenance in the cloud technology was comparatively cheaper they responded by 65% who agreed, 25% strongly agreed, 5% strongly disagreed, 4% disagreed and only 1% was neutral. As to whether the institution found it costly to maintain manual records as compared to electronic records, 51% agreed, 48% strongly while only 1% strongly disagreed. Further, on whether the electronic record system was initially costly but cheap in the long-run, 47% agreed, 35% strongly agreed, 10% strongly disagreed and 6% agreed. Only 2% were neutral. The study concluded that a unit change in X2 will increase the effectiveness of record maintenance by 0.631 units and that in the absence of cloud cost, the record maintenance will still be positive at 8.765 since there are other factors which affect the record maintenance such as network accessibility, shared infrastructure, and network security. The study recommended that the Nyandarua Institute of Science and Technology should implement its record maintenance on cloud computing technology

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Highly Sensitive Hydrogen Gas Sensor based on Fiber Bragg Grating (FBG) and Laser ablation technology

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Hydrogen gas is a recyclable, abundant, and environmentally friendly source of energy. However, its highly flammable and explosive gas at 4% limit in air.
In this research, the relationship between hydrogen concentration and peak wavelength shift of FBG optical fiber sensors were investigated and analyzed experimentally. In order to enhance its sensitivity, the fiber cladding was ablated into micro-cavities using Femtosecond laser. Ablation increased the surface area of the fiber cladding covered by hydrogen sensitive transducer. The Pt-WO3 nanolamellae prepared by hydrothermal process at molar ratio of 1:5 respectively and deposited on the surface of fiber micro-cavities. Tungsten oxide (WO3), reacts exothermically with low concentration hydrogen gas (0-0.5%) under Pt catalyst generating massive heat leading to FBG central wavelength shift. The optical sensor fabricated exhibits a high sensitivity of 170 pm/H% within the range of 0–1.4% at room temperature. This translates to approximately three times higher than the unprocessed standard FBG.

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Computational Design of a Dual Template Molecularly Imprinted Polymer

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Multi-template imprinted polymers are attractive in application in extraction and recognition of pesticide residues in environmental matrices. Computational design was used to study intermolecular interactions in the pre-polymerization mixture between methylacryamide (functional monomer) and Carbaryl and thiodicarb (templates). The interaction energies between the computer simulated template-functional monomer complexes was calculated to provide insights on the functional monomer: Template ratio of the dual imprinted polymer. The chemical structure of the template (T) molecules {carbaryl (CBL), thiodicarb (TDC) and carbendazim (CBZ)}and the functional monomer methyl acylamide (MAM) were drawn using Gauss view 5.0 and saved as Gaussian input files. The template and functional monomer were then subjected to geometry optimization at DFT level using B3LYP/6-31G(d) then subjected to optimization and frequency calculations at the same level. The frequencies were examined to ensure that the conformations correspond to a minimum on the potential energy curve. The electronic energy of the system was used for energy calculation of the complex formed. The value of change in energy (ΔE) was subsequently analyzed and used to predicts the most stable complex. The complexes exhibited negative interaction energy (ΔE) whose magnitude increased as the monomer: template ratio increases for both CBL and TDC and could be used to evaluate the imprinting process. It is observed that when higher amounts of functional monomer are used, the effect of steric crowding was exhibited by the TDC: MAM ratio 1:4 which resulted in high positive energy change that imply instability, on the other hand CBL-MAM still exhibited a large negative energy change implying greater stability. The results indicate the optimal molar ratio for the synthesis of the dual template MIP using MAM is 1: 3. The complexes of the two templates exhibited equal interaction energy at this ratio. Therefore, a computational approach can be used in designing multi-template imprinted polymers.

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Berry Curvature and Multiband formation in TaP

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Berry phase is a quantity that describes how a global phase accumulates as some complex vector is carried around a closed loop in a complex vector space.
Berry phase and related concept, usually provide a unified framework for describing many fundamental
properties of electrons in solids. By this we imply from electric polarization to quantized effects in topological materials. Tantalum Phosphide (TaP), a verified weyl semi-metal is a suitable candidate in Berryology in that many of its its intrinsic properties remain unknown. In this work, the authors will employ a class of mathematical methods that are connected to the specific geometric phases in TaP. These so called phases, are the Berry phases and they have significant roles in the band theory of electrons in TaP. We shall employ the state-of-the-art \textit{ab initio} methods as implemented in {\sc Siesta} method. The authors herein will introduce the concept of the Berry phase and explain how it enters into the quantum-mechanical band theory of electrons in crystals. As a matter of fact, we will also discuss its application to the normal adiabatic dynamics of finite quantum systems.

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Cooperative Jahn-Teller effects in ScF3

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Jahn-Teller effects arise in a crystal if distortions are considered on either the octahedral or tetrahedra complexes. This is a non-volatile approach in tailoring materials properties. ScF_3 is a material that has arouse special interests based on its Negative thermal expansion (NTE) behaviour. To this date, little is understood on the interplay between Jahn-Teller effects and NTE. The researchers herein, give a focus on how the Jahn-Teller interactions alter the chemistry of this crystal. We employed Density Functional theory as implemented in the {\sc Siesta} method coupled with mild distortions on the octahedra complex. The results herein go along way in exploring non-volatile approaches in engineering materials. Experimentalists can use this as a back bench in designing materials for novelty.
Key words: DFT, ScF3, NTE, Jahn-Teller distortions.

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Orgin of band inversion in topological Bi2Se3

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\title{Origin of Band inversion in Topological Bi_2Se_3}

\date{\today}

\begin{abstract}
Topological materials and more so insulators have become ideal candidates for spintronics and other novel applications. These materials portray band inversion which is considered to be a key signature of topology. It is not yet clear what drives band inversion in these materials and the basic inferences when band inversion is observed. We employed a state-of-the-art \textit{ab initio} method to demonstrate band inversion in topological bulk Bi_2Se_3 and subsequently provided a reason explaining why the inversion occurred. From our work, a topological surface state for Bi_2Se_3 was described by a single gap-less Dirac cone at the $\vec{k}$= 0 which was essentially at the Γ point in the surface Brilloiun zone. We realized that band inversion in Bi_2Se_3 was not entirely dependent on spin-orbit coupling as proposed in many studies but also occurred as a result of both scalar relativistic effects and lattice distortions. Spin-orbit coupling was seen to drive gap opening but it was not important in obtaining a band inversion. Our calculations reveal that Bi_2Se_3 has an energy gap of about 0.28 eV, which in principle agrees well with the experimental gap of $\approx$ 0.20-0.30 eV.
%
This work contributes to the understanding of the not so common field of spintronics, eventually aiding in the engineering of materials in different phases in a non-volatile manner.
\end{abstract}

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\end{document}

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The Interplay Of Lattice Distortion and Bands Near The Fermi Level in ATiO3(A=Ca,Sr, Ba)

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In this paper, the structural and electronic properties of ATiO3 (A=Ca, Sr, Ba) have been investigated under the strain-free situation and realistic constraints using first-principles calculations. We endeavored to find out the relationship between the interplay between lattice distortions and bandgap in three ATiO3 family members that has remained skeptical to date. The simulations were done by employing the numerical atomic orbital method as implemented in the SIESTA code. Exchange and correlation functions were treated by the generalized gradient approximation. Since only intrinsic properties of the titanates were considered in these calculations no Hubbard term to deal with the on-site Coulomb repulsion on the Ti d-states was considered. In all the calculations herein, we replaced the core electrons by ab-initio norm-conserving pseudopotentials that followed the Troullier-Martins scheme in the Kleinman-Bylander fully non-local separable representation. We found out that the electronic structure was particularly sensitive to perturbations (compressive or tensile) as expected in most materials science studies in solid state chemistry and physics. Our

results indicate that under mild strains; the bandgap (Egap), increased under compression and decreased under tension. In all the three materials, the bandgap and the lattice parameter (a) were found to relate as with 2.19< x< 3.1 for mild distortions. All these changes are attributed to the interplay of electrostatics and covalency in the crystals under study. This work acts as a yardstick on bandgap engineering to achieve desired properties in these octahedral titanates for feasible future applications in the electronics industry.

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Thermoelectric Transport Properties of Tin Selenide from First Principles Calculations

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The need for new thermoelectric materials that can be used at high temperature for large scale applications has attracted a lot of attention among the researchers over the last few decades. Tin Selenide which is lead-free and relatively cheap has become of interest in the field of thermoelectricity following the reported figure of merit value of 2.6 at 923 K along the b-axis single crystals. In this study we investigated the electronic band structure of SnSe performed using ab-initio calculations done using Quantum Espresso. Thermoelectric properties of the material between the temperature range 300K and 800K were also studied using the BoltzTrap code. Electronic structure calculations were performed using the Generalized Gradient Approximation (GGA) in the form of Perdew-Burke-Enzerhof exchange-correlation functional as implemented in the Quantum Espresso code. An indirect bandgap of 0.625eV was found compared to the experimental value of 0.9eV. Tin Selenide was found to exhibit anisotropic electrical and electron thermal conductivity as well as the Seebeck coefficient. In addition, the material's electrical and electron thermal conductivity was found to be directly proportional to temperature across all the crystal axes. Electrical conductivity was found to be higher on the a & c axes and increased significantly with temperature from 1.233×10^18 at 300K to 4.897×10^18 /Ωms at 800 K on the a-axis and from 1.416×10^18 to 6.49×10^18 /Ωms on the c axis. Electronic thermal conductivity was found to be quite low on the a-axis (8.403×10^12 W/mKs to 1.073×10^14 W/mKs). The Seebeck coefficient was found to be in the range 234 μV/K to 250 μV/K across all axes between 300K to 800K, which is sufficiently high enough for thermoelectric applications. These results show that Tin Selenide exhibits good thermoelectric properties and can perform better at high temperatures for thermoelectric applications.

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Spontaneous Polarization in BiGaO3

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It is imperative to note that at elevated temperatures, $BiGaO_3$ is a symmetric faced-centered cubic (FCC) and does not display electric polarity. As the temperature decreases, the lattice shrinks and

the symmetric arrangement is no longer stable. For instance, the Ga^{4+} cation snaps from the cube center to other minimum-energy locations situated off center. This is accompanied by corresponding motion of the O^{2-} anions. Shifting of the Ga^{4+} and O^{2-} ions causes the structure to be altered, creating strain and electric dipoles. The authors herein seek to find out the distortion ratio, also called the spontaneous strain (S_s) that will yield an electric dipole. This polar lattice arrangement forms the ferroelectric phase of the perovskite, which exists at lower temperatures and is essentially very crucial in sensors. All the calculations are carried out in the framework of density functional theory as implemented in the {\sc Siesta} method. This work is significant in the sense that it shows how a material can easily change from one ferroelectric state to another and back.

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Hole Superconductors

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Abstract: A hole is the absence of electron, and it carries a positive charge. Electrons in metals are dressed (interact with other electrons and even ions in a material) by a cloud of other electrons that surround it and interact with it. Such an interaction or dressing leads to increase in the effective mass of the electron, and the electrons in this state are called heavy electrons. The effective mass of the heavy electrons can vary between 10 mo (mo is the rest mass of the free electron) and 1000mo. thus, when the dressing is large, the metal is unable to conduct electric current and may even behave like an insulator if the heavy electrons are locked in some space in the metal. It is found that when the temperature is lowered, the electrons manage to undress and the interaction with the surrounding cloud is sufficiently reduced leading to lowering of the effective mass. This leads to easy flow of current that may be large. Creation of such large current leads to superconductivity. Such a process can occur only if the carriers in the metal in the normal state are holes and not electrons such that the undressing takes place when two hole carriers with opposite spin form a pair. When holes undress, they turn into electrons and as electrons, they behave as giant atoms resulting in a superconducting state. Hence the model of hole superconductivity demands or postulates that the mobility of holes increases with the hole concentration in the system. However, for field carrier concentration, as the temperature is lowered, the system becomes superconducting.
Keywords: Hole, Dressing, Effective mass, Heavy electrons.

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FEED FORMULATION RATIONS FOR LAYERS USING TWO-LEVEL FACTORIAL DESIGNS.

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Research has shown that about 80% of total cost of poultry production is incurred on poultry feeds. A farmer who manages to bring down this cost to about 60% to 50% will make good returns in the poultry business. In general the main objective of a firm is to maximize production thereby a good measure must be taken in formulating ration for poultry birds (chicks , broiler starter, broiler finisher, growers and layers) to ensure optimum use of resources which in turn ensure reduction in the total cost of production. If feed rations are right, the broilers will grow fast, and the layers will increase egg production at least 1 egg after every 27 hours i.e. approximately 26 eggs per hen in 30 days. To improve on the feed quality and cut down cost incurred on feeds farmers should make

should their own poultry feeds. The aim of layer diets must supply protein, carbohydrates, fats and minerals to optimize egg production, to safeguard health and maintain the desired bodyweight. This study employs the use of two-level factorial design to develop a regression model for determining optimal egg production in layers. The study uses the three main feed nutrients ; carbohydrates (80% to 85%), proteins (13% to 15%) and minerals (1.5% to 2.5%). The design points were replicated twice and the average number of eggs per hen in 30 days were used. The analysis of variance table showed the main effects carbohydrates, protein and minerals are significant, carbohydrates and proteins, carbohydrates and minerals interactions were also significant. A plot of residuals versus the predicted values appeared satisfactory so we have no reason to suspect problems with validity of our conclusions.

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Synthesis, Characterization of ZnO Nanoparticles and their Application in Removal of Heavy Metals from Waste water

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In an effort to reduce the environmental and health effects of heavy metals in wastewater, various techniques have been employed. However, most of these techniques are expensive and ineffective incomplete removal heavy metals from the waters.The objectives of this study were to synthesize ZnO nanoparticles, characterize and apply it in adsorption of heavy metals from waste waters. Precipitation technique was used to synthesize ZnO nanoparticles. Two samples L1 and L2 were synthesized. They were characterized using Power X-ray Diffraction (PXRD), Fourier Transform Infra-Red (FTIR), Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray Spectroscopy (EDX), methods of analysis. The PXRD results showed diffraction peaks which were indexed to ZnO reference as per JCPDS file 80-0075. The size of ZnO nanoparticles was found to be 26 nm. FTIR spectra showed a broad band at around 430 cm-1 with shoulder shape, characteristics of Zn-O bond. The images obtained by SEM showed rod shaped clusters of nanoparticles which were distributed well within a range of 100 nm which is a favorable property to exhibit better photo catalytic activity. The EDX results showed elemental composition of ZnO nanoparticles which showed 54% Zn, 44.07% O and 1.93% Mn impurities for L1 and 55.34% Zn, 42.3% O and 2.37%Mn impurities for L2.The results of heavy metal ions adsorption showed an increase in percentage removal with increase in adsorbent dose and contact time. There was a decrease with increase in heavy metal concentration. In conclusion, ZnO nanoparticles can be used an adsorbent of waste water from textile and metallurgical industries. Future studies could focus on possibilities of improving and commercializing this material through designing a treatment facility that in co-operates commercial nanoZnOon large scale waste water treatment.
Key Words: Heavy Metals, Adsorption, ZnO Nanoparticles.

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Comparative Study on the Accuracy of Selected Solar Radiation Models Against Measured Data Under Tropical Climate

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Abstract
Availability of high accuracy time-series solar radiation data is of primary importance in the prediction of energy produced by solar energy conversion devices. Since performance of any solar energy

system is site-dependent, it is beneficial if local operating conditions are known at the planning stage. Unfortunatîely, ground-based measurements of solar radiation are lacking in most locations where solar appliances are installed due to high cost and maintenance of the solar radiation measurement equipment. To overcome this limitation, solar radiation data can be obtained by several sources such as numerical weather prediction models, satellite base forecast, all sky images and ground measurements at nearby public weather stations. However, these data are characterized by the type of data they produce and spatial-temporal granularity, hence generated data may be more or less accurate at the application site given the variability of the weather phenomena. Numerical radiation models are widely used to estimate solar radiation, but need to be validated by high-quality solar radiation data measured at different climates in order to improve their accuracies. In this work, comparison of one year solar radiation data measured using a reference solar cell at a location in western Kenya with the corresponding data generated from four selected models are presented. Reasonable agreements between measured and modeled data were realized with absolute uncertainties of 12.6%, 8.5%, 15.5% and 11% for Hargreaves-Samanni, Angstrom, Iqbal, and ASHRAE models respectively. Hence, the Angstrom model yields more accurate prediction of solar radiation at the site compared to the other models.
Keywords: Solar, irradiance, data, measurement, model, devices.

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Ab Initio Study of Mechanical Properties of Lead Halide Perovskite For Photovoltaic Application.

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The ever increasing demand for energy has necessitated the need of coming up with measures of seeking alternative energy sources. Solar energy is one of the most important alternative sources of energy. The use of the first and second generations solar cells made of silicon in making solar panels has notable shortcomings such as unaffordability and lack of longevity of the electric power generated. In this regard, we report the mechanical properties results of lead halide perovskite (ABX3) where (X = I/Br/Cl , A=CH3NH3/CH(NH2)2+/Cs+ and B can be divalent metal ion for example (Pb2+, Ge2+, or Sn2+).Calculations were done using density functional theory within generalized gradient (GGA) approximations, using norm-conserving pseudopotentials generated from the Troullier-Martins scheme. Elastic constants calculated in this work include as bulk modulus B, Young's modulus E, shear modulus G and Poisson's ratio ν were calculated using the Voigt–Reuss–Hill averaging scheme. The Poisson's ratio ν obtained was 0.25 which is close to the experimental value of 0.28, this value confirms that CH3NH3PbI3 is a ductile material. The result from the elastic constants done compares well with previously done work. A ductile material can be moulded to different shapes and size, therefore CH3NH3PbI3 is suitable to be used as a photovoltaic material.