Kabarak University International Conference on the Basic Sciences 2019

Report of Contributions

Contribution ID: **3** Type: **Abstract for Research Paper**

STRUCTURAL PROPERTIES OF PHOTOCATALYTIC COPPER PIGMENTED ANODIZED TITANIUM

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Titanium dioxide (TiO2) photocatalysis is an advanced oxidation process with key advantages over other water treatment technologies including the lack of mass transfer limitations, operation at ambient conditions and the potential use of solar radiation. In this study, commercial pure grade 1 titanium substrate was anodized at 200V for different anodization times, pigmented and annealed for a period of 450 0C for 4 hours. Structural properties of the samples was done using AFM, XRD and SEM. Prolonging anodization time engineered the formation of pores and pores merging of the TiO2 film thereby significantly influencing the surface morphology and crystallinity of the sample. The XRD measurements confirmed the coexistence of both rutile and anatase phases in the samples.

Keywords

Keywords: TiO2, Photo-catalysis, anodization, pigmentation, structural properties.

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Track Classification: Emerging and cross-cutting issues in the Basic sciences

Contribution ID: **4** Type: **Abstract for Research Paper**

ab initio studie of the effect of dopant scandium on mechanical and electronic properties of zinc oxide

Zinc oxide has attracted great interest in the last few years. This is because electronics based on ZnO have wide applications and better performance on account of improved electronic conductivity, lower power consumption, better stability, fast electron transfer kinetics and improved storage capacity. ZnO crystals are able to withstand much higher electric fields than silicon crystals, such that electronic devices based on ZnO will be able to operate on higher power and higher temperature. The main drive globally is to come up with a cheap and reliable photovoltaic source. ZnO is one of the materials that can be investigated to come up with such materials. Electrical conductivity of ZnO is enhanced by doping with other suitable elements. The effect of doping indium, aluminium, yttrium and gallium in ZnO has been frequently reported by various groups but effect of rare earth metals such as scandium has scarcely been reported. The objective of this research is to study the mechanical and electronic properties of dopant Sc on ZnO using ab initio study. The main method is based on using quantum espresso code and interactive solution of the Kohn Sham equation of density functional theory in a plane wave set. From the data obtained, the band gap reduced after doping ZnO with scandium. This will therefore make the final product a highly conductive and transparent film that can be used in solar cells

Keywords

scandium,doping,zincoxide

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Track Classification: Computational Modelling of Materials

Contribution ID: **5** Type: **Abstract for Research Paper**

AB INITIO STUDY OF STRUCTURAL AND ELECTRONIC PROPERTIES OF B-DOPED SnO2

ABSTRACT
Conventional energy sources such as crude oil and fossil fuel have negative effects on the environment mainly due to pollution necessitating the development of alternative energy sources. Silicon based technology has been extensively used in solar cells, but is very expensive. SnO2 film has proved to be best material for fabrication of solar cells because it is non-toxic, abundant, is thermally and chemically stable, and has low cost hence making it an efficient converter of solar energy to electrical power with low cost of production.This study is an ab initio study of structural and electronic properties of pure and boron doped trivalent element B(x=0, 0.625, 0.125) in SnO2 thin films using Full- Potential Augmented Plane Wave (FP-LAPW) method based on density functional theory as implemented in the Quantum ESPRESSO code.The structural and electronic results indicated that as the Boron concentration increased in rutile tetragonal SnO2, lattice parameters decreased (0.01 Å and 0.02 Å and for c are 0.02 Å and 0.038 Å) and band gap increased (2.84 ~ 3.17 eV). Fermi level shifted into valence band and material tend to convert into p-type semiconductor.

Keywords

B-doped SnO2, Transparent conducting oxide, Low reflectivity, Band gap

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Track Classification: Emerging and cross-cutting issues in the Basic sciences

Contribution ID: **6** Type: **Abstract for Research Paper**

Optical characterization of Cobalt pigmented ZnO films fabricated by anodization for photocatalytic water purification.

While the sixth sustainable development goal to be achieved by 2030 is clean water and sanitation, there is still a global challenge in the supply of adequate clean water due to population growth and urbanization. This necessitates coming up with more affordable approaches of managing waste water. Photocatalytic degradation of pollutants has proved to be one of the promising ways of purifying water. This study aimed at preparing Cobalt doped ZnO films to be used in photocatalytic water purification. ZnO films were fabricated by anodization and Cobalt incorporated. Heat treatment was done at 2500C. Optical characterization was done using a UV-VIS NIR spectrophotometer in the solar range 300nm – 2500nm to obtain reflectance data which aided in determining the optical properties of the films. Data analysis showed a decrease in ZnO reflectance and optical band gap on incorporation of Cobalt. This implied an increase in the absorption of the films which is a fundamental property in photocatalytic water purification. Hence Cobalt doped ZnO films have good photocatalytic properties and can be used for photocatalytic water purification.

Keywords

ZnO, anodization, photocatalysis, heat treatment, doping

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Track Classification: Emerging and cross-cutting issues in the Basic sciences

Contribution ID: **7** Type: **Abstract for Research Paper**

AB INITIO STUDY OF ELECTRONIC PROPERTIES OF LEAD HALIDE PEROVSKITES FOR OPTICAL PERFOMANCE OF SOLAR CELL

ABSTRACT
The ever increasing demand of 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. However,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, therefore, we report the initial electronic structure results of lead halide perovskite (APbX3) where (X = I/Br/Cl and A=CH3NH3/CH(NH2)2+/Cs+) for application in solar cells. The density functional theory investigations was done using Pwscf code from Quantum espresso and calculation of the electronic properties of lead halide perovskites done to predict its suitability in photo voltaic applications. The current calculated results of lattice parameter and band gap of this material is in agreement with other reported calculations from experimental and theoretical studies. Mechanical properties are also reported and compared with other studies.
Key words; Electronic properties, optical properties, solar cells

Keywords

Electronic properties, optical properties, solar cells

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Track Classification: Computational Modelling of Materials

Contribution ID: **8** Type: **Abstract for Research Paper**

Towards a Unique, Secure, and Robust Wireless Local Area Network Device Identifier

With today's technological evolution, wireless networks have become very common for organizations, homes and public places. For any device to be authenticated and authorized to use any of the wireless network services, it must first be identified then authenticated and authorized to have access to the wireless network resources. One of the biggest challenges with implementing wireless networks, though, is implementing the identification of the wireless devices. Apart from port numbers and IP addresses at application and network layers respectively, devices in a network use MAC addresses for identification at the physical layer. However MAC addresses can be spoofed and altered thereby compromising the security, robustness and uniqueness qualities of a device identifier. This study therefore examined uniqueness, security and robustness characteristics of MAC in relation to a device serial number in order to establish a suitable network device identifier. In order to achieve this, test runs through a proof of concept method by using Advanced IP Scanner and getmac command line tools. Advanced IP Scanner was used to spoof MAC and serial number of a device to determine the security, hence robustness of the identifiers while getmac was used to determine uniqueness of the identifiers. The run tests indicated that a MAC address can actually be spoofed and altered rendering the MAC address not unique, insecure and unreliable. This is as a result of the fact that a computer's MAC address, apart from it being hard-coded in the hardware, has a copy of the MAC address in the system software. On the contrary, a computer's serial number is hard-coded in the hardware only and therefore cannot be spoofed and altered making it unique, secure and reliable. The researcher recommends that a study be conducted on how a device serial number can be used as network device identifier

Keywords

Network device, MAC Address, Serial Number, Identifiers, Wireless Local Area Network

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Track Classification: Emerging and cross-cutting issues in the Basic sciences

Contribution ID: **9** Type: **Abstract for Research Paper**

The physics of strongly correlated systems: A dynamical mean field theory approach

To this date, first-principles Density functional theory (DFT) has proven successful in the study of electronic structure of real materials. At the same time, we have plenty of program packages in which first-principles DFT has been implemented and are able to calculate material properties accurately and efficiently. However, the authors here in are concerned with the strongly correlated materials, where the electron-electron interaction heavily influences the electronic structure. It is a well known problem that first-principles DFT fails in describing these types of materials correctly. The reason for this failure is that first-principles DFT only includes electron-electron interactions in an average way. Many attempts have been proposed to solve this discrepancy. Among them is the inclusion of the Hubbard model in the electronic structure calculations. After working on many systems and more specifically ferroelectrics, we have faced some challenges posed by the Hubbard model in our day to day calculations. One, the calculation ceases being a first-principle to a semi-empirical like in the sense that you have an extrinsic energy in the system (DFT+U). Secondly, the application of the Hubbard model makes some systems loose their intrinsic properties like ferroelectrity. A good example is the loss of the O $2p$ and Ti $3d$ hybridization in $BaTiO_3$ when the Hubbard model is employed and thus rendering $BaTiO_3$ a paraelectric. In this work, the authors will highlight the recently developed dynamical mean field theory (DMFT). In principle, DMFT originates from the many-body approach in computational materials physics. DMFT has been combined with conventional DFT methods to help us conceptualize the physics of strongly correlated systems.

Keywords

DMFT, first-principles, Density functional theory

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Track Classification: Computational Modelling of Materials

Contribution ID: **10** Type: **Abstract for Research Paper**

Tantalum phosphide: A topological weyl semimetal.

Topological semi-metals are newly discovered states of quantum matter that have arose interest in the research community due to their application in spintronics and valleytronics. There are three types of topological semi-metals (TSMs); Dirac Semi-metal (DSM), Weyl Semi-metal (WSM) and Node Line Semi-metal (NLSM), each with special features that makes them novel candidates for future technologies. Unlike topological insulators (TI) that have an energy gap, TSMs have their valence and conduction bands touching in discrete points in the Brillouin zone. Tantalum phosphide (TaP), has been classified as a weyl semi-metal with only a single type of Weyl fermions and thus topologically distinguished from tantalum arsenide (TaAs) that has two types of Weyl fermions. Theoretically, if spin-orbit interaction is turned on in the system, we expect an energy gap. To this date, little has been devoted on this relativistic interaction in TaP. Our goal will be to calculate the bandstructure in TaP and how the spin-orbit interaction alters the single Weyl fermions. We will employ first-principles density functional theory (FPDFT) as implemented in SIESTA code. This study is not only based on fundamental research interests but also of great potential for future applications.

Keywords

TSMs, WSM, first-principles, Density functional theory.

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Track Classification: Computational Modelling of Materials

Contribution ID: **11** Type: **Abstract for Research Paper**

A First principle Study of the Power Factor of phosphorus nitride – a binary Skutterudite

Waste heat generated in most domestic and industrial appliances can lead to fracture or undesirable plastic deformation of materials. Developing new thermoelectric materials or improving the existing ones could be handy in minimizing waste heat. Skutterudites exhibit good electrical and modifiable thermal conductivities making them to be suitable candidates for thermoelectricity. Studies have hinted that skutterudite phosphorus nitride is potentially a thermolelectric material but details remain scanty to date. For more than half a century, emphasis has been placed on the figure of merit (ZT) to pinpoint good thermoelectric. Recently, it has been shown that a material's power factor is more important than the thermal conductivity for thermoelectric power generation for a given ZT. In this work, will calculate the power factor of phosphorus nitride to ascertain its thermoelectric capability. This will be investigated by solving the Boltzmann transport equations using the BoltzTraP code. It is hoped that the outcome of this study may contribute to a better understanding of properties that enhance the efficiencies of thermoelectric materials.

Keywords

Skutterudite, power factor

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Track Classification: Computational Modelling of Materials

Contribution ID: **12** Type: **Abstract for Research Paper**

Mechanical Stability of Beryllium chalcogenides: BeX (X= S, Se, and Te)

Beryllium chalcogenides (BeX) are semiconductor materials which belong to the family of II-IV semi-conductors. They manifest in four-fold coordinated zinc-blende structure at 0GPa and 0K DFT conditions which is unique in the chalcogen family. These compounds have many useful technological applications yet some properties are yet to be explored due to their toxicity and thus the ab initio methods are recommended. All calculations in this work were done based on Density Functional Theory (DFT) framework and a plane wave basis set as implemented in the quantum ESPRESSO computer code. The projector Augmented Wave pseudopotentials were used to describe core valence electron interactions with the GGAs and LDA chosen as the exchange correlations. A comparison with previous DFT work and experimental work was also done. The calculated values of the lattice parameters agreed with the experimental ones and only varied by 0.1\%. The bulk modulus obtained from pz was found to high due to its known effect of overbinding the lattice parameter. The other mechanical moduli agreed with the existing experimental and theoretical data and there was clear indication that all beryllium chalcogenides are brittle except BeTe that was ductile. The rich mechanical properties of these chalcogenides informs the suitability of these compounds for optical use.

Keywords

chalcogenides; elastic properties; Density Functional Theory

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Track Classification: Computational Modelling of Materials

Contribution ID: **13** Type: **Abstract for Research Paper**

Bandstructure of Indium and Tin doped $AgAlS_2$

Previous studies of chalcopyrites as absorbers for intermediate band solar cells (IBSC) mainly focused on Cu-based compounds, whose intermediate band is usually empty due to its intrinsic p-type conductivity. $AgAlS_2$ chalcopyrite belongs to a group of direct band gap semiconductors with novel applications in optoelectronic devices. Theoretical studies have hinted the possibility of using $AgAlS_2$ in IBSC due to the fact that its large bandgap can be easily tuned. To this date, this recommendation has not been attempted. It is for this reason that we will carry an *ab initio* study on $AgAlS_2$ to ascertain this prediction.
We will employ the state-of-the-art first principles density functional theory (DFT) as implemented in the quantum ESPRESSO computer code to calculate the bandstructure of tetragonal $AgAlS_2$. The bandstructre of $AgAlS_2$ will be determined along $\Gamma\ M\ P\ PA\ X$ high symmetry points in the Brillouin zone.
Substitutional doping using tin/indium as dopants will be done using the supercell technique $(2 \times 2 \times 2)$ on the trivalent cation site with varying concentrations until a band gap of ≈ 2.4 eV is obtained. This gap is carefully chosen since it is ideal for IBSC. This project is not only for academic purposes but it is also handy in designing solar cells with high efficiency and cost effectiveness.

Keywords

$AgAlS_2$, first-principles, Density functional theory, IBSCs.

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Track Classification: Computational Modelling of Materials

Contribution ID: **14** Type: **Abstract for Research Paper**

USING THE DIELECTRIC CONSTANT OF COMBINED DRUDE AND LORENTZ TO MODEL THE OPTICAL PROPERTIES OF SnO2: F FOR SOLAR ENERGY APPLICATIONS

Optical coatings have a variety of applications some of which include: -: transparent heat mirrors, antireflection coatings, architectural coatings, photo-thermal converters, photovoltaic converters and photo- catalysis. SnO2: F films are widely used for solar cell applications as the front electrode as well as other applications such as electrochromics and displays. Optical design of these and other applications need the knowledge of optical constants. In this study we used the dielectric constant of a combined Drude and Lorentz to model the optical behavior of SnO2: F. To do this, we used the fitting parameters from existing literature. From the model we got n and k values which we inserted into Fresnel R and T calculator and computed R and T spectra using Fresnel's equations. The effect of the thickness-dependence and carrier concentration of SnO2: F on parameters such as refractive index (n), extinction coefficient (k), real part and imaginary part are also studied. We plotted n, k, T and R for different values of plasma frequency, and damping parameter, .

Keywords

Optical constants, damping parameter, thin film and Drude-Lorentz model.

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Track Classification: Emerging and cross-cutting issues in the Basic sciences

Contribution ID: **15** Type: **Abstract for Research Paper**

CsGeI 3 , a Ge-based perovskite halide with Photovoltaic capabilities

Photovoltaic solar cells (PSCs) have undergone a metamorphosis by adopting the halide perovskites with a chemical formula of ABX3. The ABX3 PSCs have arose a lot of research interests due to their high power conversion efficiency (PCE) of ≈22%. Traditionally for a long time, PSCs were based on hybrid organic-inorganic iodide CH3NH3PbI3, but due to the toxic Pb and its chemical instability, it posed both environmental and large-scale commercialization threats. To address these challenges, researchers opted for composition tuning using nontoxic Sn2+ or Ge2+ for Pb2+ and inorganic Cs+ or Rb+ for the organic part in CH3NH3PbI3. Unfortunately, Sn-based perovskite photoabsorbers have been associated with coarse efficiency due to the large mismatch of band alignment between them and charge carrier conductors. The other detriment of the Sn-based perovskites is the susceptibility of Sn oxidation from +2 to +4 state upon exposure to air and this has slowed research efforts in Sn-based PSCs. It is for the above-mentioned reasons that Ge-based inorganic perovskites, have stood out as the best alternatives for the Pb free and long term PSCs. It has been reported experimentally that CsGeI3 stabilizes in the rhombohedral phase with R3m space group at room temperature and theorists have equally tested its structure formidably by analyzing its Goldschmidt tolerance factor. Here in, we will perform a theoretical investigation based on state-of-the-art density functional theory (DFT) as implemented in the quantum ESPRESSO computer code, to get a comprehensive understanding of CsGeI3 for solar cell applications. The structural and optoelectronic properties of inorganic CsGeI 3 halide perovskite will be calculated by the use of PBEsol functional without SOC effect. This project will guide experimentalist in designing novel PSCs for future technologies. We also recommend other studies to be conducted when Cs is replaced with Rb so as to get better PSCs.

Keywords

PSCs; CsGeI 3 ; Density Functional Theory; opto-electronic

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Track Classification: Computational Modelling of Materials

Contribution ID: **16** Type: **Abstract for Research Paper**

Equation of state for a 2D system

We have described a simple theoretical model of an equation of state (EOS) for a two-dimensional system. The goal was to give a clear description of the interplay between hydrostatic change in surface area and the two dimensional in-plane pressure (F). Of interest from this described EOS, was the measure a material's resilience to isotropic stretching (γ) that can in principle be viewed as the layer modulus. To this date, few attempts have been made to obtain accurately the layer modulus of 2D systems. We studied using density functional theory as implemented in the {\sc SIESTA} computer code, a number of monolayer systems; graphene, boronitrene, dichalchogenides and janus chalcogenides. The results found out in this study showed that of the above honeycomb structures, graphene was the most resilient to stretching with a value of $\gamma_C = 206.6\ N/m$ followed by boronitrene $\gamma_{BN} = 177.3\ N/m$. The layer modulus of the dichalcogenides and janus chalcogenides was seen to be competing but not as large as that of graphene or boronitrene. Apart from the layer modulus, we were also able to use the EOS to predict isotropic intrinsic strength of the listed systems. It was observed that the instrinsic stress was proportional to the layer modulus. This project does not just satisfy our knowledge thirst but can also be used by experimental groups in fabricating hard 2D materials.

Keywords

EOS, first-principles, Density functional theory, layer modulus.

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Track Classification: Computational Modelling of Materials

Contribution ID: **17** Type: **Abstract for Research Paper**

Effects of solvent polarity on the absorption and fluorescence spectra of 3-cyano-7-hydroxy-4-methylcoumarin: determination of the dipole moments and application to epifluorescence microscopy.

Abstract

The Absorption and fluorescence emission spectra of 3-cyano-7-hydroxy-4-methylcoumarin (3C7H4M) were studied in solvents of different dielectric constant ε and refractive index n. Experimental ground and excited state dipole moments were established by means of solvatochromic shift method. Both the ground state and excited state dipole moments were. Results revealed that the excited state dipole moments of 3C7H4M were higher than those of the ground state. Further it is evident from these results that, the changes in the dipole moments on electronic excitation are small. Since 3C7H4M is more polar in its excited state, polar solvents were chosen in epifluorescence study. The epifluorescent microscopy images of a plant cell stained by 3C7H4M in various polar solvents compared with Iodine are hereby reported.

Keywords

dipole moments, epifluorescence microscopy, spectral shifts

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Track Classification: Emerging and cross-cutting issues in the Basic sciences

Contribution ID: **21** Type: **Abstract for Research Paper**

Pressure dependence of elasticity in α-TiZr shape memory alloys

Abstract
Shape memory alloys are a group of materials with two noteworthy properties; shape memory effects and superelasticity thus they have attracted a number of industrial applications. Elasticity is the ability of a material to resume its normal shape after being stretched or compressed when the elastic limit is not exceeded. Titanium Nickel, copper-based and iron-based shape memory alloys are mostly applied in constructions sector but they face challenges of pressure dependency. To provide a solution, we investigated the pressure dependency of elasticity in α-TiZr shape memory alloy. Elastic constants, bulk modulus, Young modulus, shear modulus and Poisson's ratio of α-TiZr shape memory alloy were calculated at different pressure (0-10GPa) using Quantum ESPRESSO code with post-processing of the data done using Thermo_pw code. Projector augmented wave pseudo-potential with Generalized Gradient Approximations (GGA) within Perdew, Burke, and Ernzerhof (PBE) exchange-correlation functional was applied in this study. A compressive study of pressure dependency of elasticity in α-TiZr shape memory alloy is meant to avail information which may lead to adoption of this alloy in construction of intelligent reinforced concrete (IRC). Shape memory alloy wires incorporated in concrete of buildings and bridges Shape memory alloys can sense cracks and contract reducing large scale sized cracks therefore our buildings and bridges will become dynamic and sensitive to the outside changes.

Keywords

α-TiZr, Elasticity, Density functional theory

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Track Classification: Computational Modelling of Materials

Contribution ID: **22** Type: **Abstract for Research Paper**

Optical capabilities in copper oxides, a density functional study

Copper oxides have attracted a lot of interest due to their photo-catalytic applications in solar cells, water splitting and CO 2 reduction. They are novel candidates to provision of clean renewable routes to fuels. These processes require that copper oxides should have a higher solar conversion efficiency which is to this date reported to be low for cost-effective applications. Previous studies hint the possibility of lattice distortions on Cu 2 O and CuO to boost their optical capabilities but details on their photo-absorption in the distorted regime are still unclear and thus limited applicability. The authors here in employ the state-of-the-art ab initio methods to study the photo-absorption in Cu 2 O, CuO and Cu 4 O 3 for solar cells applications. All the calculations will be done in the density functional theory (DFT) framework as implemented in the Quantum ESPRESSO package. Post-processing of the preliminary data will be done using the Yambo code that solves the Bethe-Salpeter equation to obtain the optical absorption spectra. The findings in this work are expected to enhance photo-response in copper oxides for solar cells applications.

Keywords

Key Key words: copper oxides, first-principles, Density functional theory.

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Track Classification: Computational Modelling of Materials

Contribution ID: **23** Type: **Abstract for Research Paper**

Structural and mechanical properties of BP3N6

Using first-principles calculation, the structural and mechanical properties of BP3N6 which adopts an orthorhombic structure with space group Pna21 (no. 33), were determined at three different pressure values (0, 20 and 42.4 GPa). The nine independent elastic constants meet all necessary and sufficient conditions for mechanical stability criteria for an orthorhombic crystal. BP3N6 show strong resistance to volume change hence a potential low compressible material. The Vicker's hardness of BP3N6 was found to range between 49-51 GPa for different external pressures imposed on the crystal. These high values of Vicker's hardness imply that BP3N6 is potential superhard material.

Keywords

boron phosphorus nitride; DFT; Vickers hardness.

Primary author: Dr MANYALI, George S. (Masinde Muliro University of Science and Technology)

Track Classification: Computational Modelling of Materials

Contribution ID: **24** Type: **Abstract for Research Paper**

High Performance Computing in Materials Science

Computational modeling in materials science involves the employment of fundamental physical and life sciences as well as computer science to study the properties of matter at the microscopic level. Such studies can be carried out by electronic or atomistic approaches and the outcomes used to complement the applied sciences as well as to guide experimental research work. Over the last decade, affordable computing resources coupled with community developed state-of-the art codes are available for graduate students and research staff even in the developing world, where there is limited funding. This has been made possible through collaborative research or via initiatives from friendly partners in Europe and America. It is therefore possible to engage in quality research for capacity building or the development of products and services. Computational modeling can now predict, independently, outcomes of some materials properties to within accuracies of less than 5% compared with independent experimental techniques. This implies that computational modeling can be used as a decision support tool, enabling tests before production, hence cutting down costs from the previous trial and error approaches. Current problems in science and technology require a multidisciplinary approach such as that being employed in computational modeling and hence its applications in both fundamental and applied sciences. Due to the accessibility of resources to perform research using computational modeling in materials and other applied sciences, additional effort needs to be made to involve more graduate students and faculty in these areas for capacity building. In due course, it is expected that the research capacity realized will be focused to solve current and emerging problems in this country.

Keywords

High Performance Computing, Materials Science

Primary author: AMOLO, George (The Technical University of Kenya)

Track Classification: Computational Modelling of Materials