KABARAKUNIVERSITY

INTERNATIONAL CONFERENCE ON MATHEMATICAL, PURE & APPLLIED SCIENCES 2023

THE BOOK OF ABSTRACTS

Editor:

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July 10 – 11, 2023

Contents

Conference Programme

Day One: 10th July 2023

REGISTRATION

Session Chair: Professor C.M. Maghanga

TIME	ACTIVITY	FACILITATOR
8.00– 8.30 AM	Registration	Ms. Sharon Cherotich
8.30– 8.40 AM	Meditation	Rev. Prof. Jacob Kibor, Provost
8.40– 8.50 AM	Welcoming Remarks	Prof. Maghanga Christopher
8.50–9.00AM	Opening Remarks	Dr. Peter Rugiri, Dean School of Science, Engineering & Technology
9.00– 9.05 AM	DVC(A&R)	Prof. John Ochola
9.05 – 9-20 AM(FLEXIBLE)	Welcome remarks by the Vice Chancellor	Prof. Henry K. Kiplangat
9.20– 10.00 AM	Keynote Address	Prof. Mghendi Mwamburi
10.00– 10.40 AM	Guest Speaker	Dr. Paul Njogu
10.40– 11.20 AM	Guest Speaker	Prof. K. M. Khanna
11.20– 11.25 AM	Vote of thanks	DR. Moses Thiga
11.25– 11.55AM	**Tea Break and Move To Breakout Rooms**	

Chair: Dr. Peter Tanui
Rapporteur: Ms. Gladys Kwemoi

PAPER	PRESENTER	TIME
01 Piezo – Photocatalytic Performance of Fe- Doped $BaTiO_3$ Compounds	Wycliffe M. Isoe, Maxwell J. Mageto, Benjamin V. Odari, Onesmus M. Munyati, Maurice M. Mwamburi, Christopher M. Maghanga, Sylvester Hatwaambo	12.00 – 12.20

02 Influence of WO_3 doping on Optical Properties of SnO_2Thin Films Synthesized by Sol-gel Spin Coating Technique	Victor Isahi, Christopher Maghanga, Mghendi Mwamburi, Onesmus Munyati, Sylvester Hatwaambo, Emmanuel Akoto, Wycliffe Isoe, Mir Waqas Alam	12.20 – 12.40
LUNCH BREAK		**12.40 – 2.00 PM**

Chair: Winnie Bor
REPORTEUR: Ms. Sharon Chemutai

PAPER	**PRESENTER**	**TIME**
03 Electronic Structure, Mechanical and Dynamical Properties Study of Strontium Doped Barium titanate; $Ba_{1-x}Sr_xTiO_3$ Perovskite; A First Principle Study	P.W.O. Nyawere and D. N. Maina	2.00– 2.20 PM
04 Thermodynamic parameters for hydrogen storage in metal organic frameworks	Hezekiah K. Cherop and Jason B. Kanule	2.20– 2.40 PM
05. Structure and properties of superconducting Magic Angle Twisted Bilayer Graphene	Peter TANUI and Dismas KIBOI	2.50– 3.15 PM
06 Bayesian methods in Medical Research: The case of Survival Models	Henry Ondicho Nyambega	3.15– 3.35 PM
07On Mutual class (Q) operators	Wanjala Victor , John Wanyonyi Matuya and Edward Njuguna	3.35– 3.55 PM
TEABREAK		**3.55 – 4.15 PM**
08*Ab initio* high pressure study of semiconductor-metalphase transition of the chalcogenide compound $KPSe_6$	Ogwoka P.J, Otieno C.O and P.W.O. Nyawere	4.15– 4.35 PM
09Developmentofanau tomatedhalleffect experimentation	A. Orega, M. Mwamburi, C. Maghanga	4.35– 4.55 PM

method for the electrical characterization of thin films		

DAY TWO: 11th July 2023
Chair: Mr. Robert Rotich
Rapporteur: Mr. Chepkok

PAPER	**PRESENTER**	**TIME**
DEVOTION	**DRNYAWERE**	**8.30 –8.40 AM**
10.Tungstendoped TiO2 fororganic dye removal from wastewater	Gloria I. Murila, Maxwell Mageto, Mghendi Mwamburi, Samiji Margaret	8.40– 9.00 AM
11.Mechanical Properties of Al-Mg-Si Alloys (6xxxSeries):ADFT-Based Study	Pius Kipkorir, Nicholas Ongwen, Maxwell Mageto, Victor Odari, Francis Gaitho	9.00– 9.20 AM
12. Expanding the Scope of Computational Alchemy for Efficient Screening of Non-Noble Transition Metal-Doped Pt Catalysts for CO_2 Reduction	Cecil Ouma	9.20– 9.40 AM
13. Chi Square Modeling on challenges facing Kenyan University Students	Monari	9.40– 10.00 AM
TEABREAK		10.00– 10.30 AM
14.Influence of the Substrate Temperature and Ag Incorporation on the Properties of Reactively DC Co-Sputtered Ag:TiO_2 Thin Films	Hezekiah Buay Sawa, Margaret Emanuel Samiji, Nuru Ramadhani Mlyuka	10.30– 10.50 AM
15. The modelling of photovoltaic characteristics of Lead – freeCs1-RbxSnI3 – silicon tandem solar cell: modelling of photovoltaic characteristics of lead – freeCs1-xRbxSnI3 – silicon tandem solar cell	Emmanuel Akoto, Victor Odari, C. Maghanga	10.50– 11.10AM
16.The role of weather parameters on a solar system performance	Sebastian Waita and Rita Mwende	11.10– 11.30AM

Keynote Address 1

Professor Henry Kiplangat
The Vice Chancellor, Kabarak University

It gives me great pleasure to welcome you to our 3rd Annual International Research Conference of the year 2023 and specifically to the Conferences;

1. Mathematical, Pure and Applied Sciences Conference event jointly hosted by the School of Science, Engineering and Technology, and the School of Education and
2. Environment and Energy Conference of School of Science, Engineering and Technology

Guest Speaker, dean, attendees and all protocols observed, good morning and welcome to the two Kabarak University International Conferences. This year our conferences are blended (online and face to face) and we appreciate all participants and attendees for creating time to be with us in these two days conference whose theme is "*Bridging Research Gap through Basic and Applied Sciences"* for Mathematical, Pure and Applied Sciences Conference and *"Sustaining Resource Utilization and Energy Efficiency"* for Environment and Energy Conference.

The two conferences are held together this year because they are hosted by two schools but their contents are similar. While conference one on Mathematical, Pure and Applied Sciences is on hard sciences; conference two on Environment and Energy is on applications of these sciences.

As a university we have endeavoured to create an environment conducive for both research and learning experiences. We have had collaborations with likeminded institutions and industries to enable exchange of skills. In particular, School of Science Engineering and Technology in the recent past have had collaborations with;

1. Microsoft which was done in January 2023
2. Safaricom done in June 2023
3. Power to Learn which was done in February 2023
4. Huawei collaboration which was recently renewed for hosting of Huawei Academy.

The school has also competed and won different trophies including;

1. The Best Stand in Embracing ICT Systems Education Position 1 at Nakuru ASK Show 2022
2. The Best in Presentation of Latest Technologies in Internet of Things (IOTs) and Artificial Intelligence 2022.

It is also important to note that ICT Authority of Kenya; North and South Rift Region has chosen Kabarak University as a centre of training and two staff members of the school of SSET are currently being trained so that they can also train others.

Recently a workshop on Internet of Things (IOTs) and Robotics for students of Computer Science, IT and Forensics was hosted by the school. The following Robotics were displayed by the students;

a.) Control of conditions of a greenhouse
b.) Dancing Robotics
c.) Factory Control Machines
d.) Smart Car
e.) IOT – Base Air pollution monitoring system

These are but a few of the achievement of the school and I believe we are at a position of using technology to provide solutions to challenges we are encountering socially, technologically or even academically. To provide necessary scientific solutions, there is need for research output in hard and applied sciences. My administration has endeavored to provide an environment necessary for research and we have supported these and other conferences to show case our research. We have provided resources in terms of reading materials both physical and electronically to enhance availability of information to our researchers. Subscription to world class journals through our Library has made search for information and publications easier and faster. We have also provided a faster internet connectivity across our campus which enables both staff and students to comfortably access the necessary information for their consumption.

It is therefore expected that some of the outcomes of our research work presented here on computational simulations and data from some of experimental work in both physics and chemistry will play a role in helping national policy makers come up with relevant policies in regard to funding of these programmes. With proper funding and collaboration between universities and industries, new materials simulated can be fabricated for application in areas such as biophysics, medicine, solar panels just to mention a few. This collaboration is currently encouraged through National Research Fund (NRF) agenda where various universities on similar or different areas of specialties can be funded to do research together.

On energy, the critical challenge is to limit the effects of global warming while maintaining a balanced economic growth. The impact of global warming mitigates the fundamental problem while ensuring the balance economic development. Intense research efforts should be directed toward balanced resource utilization, renewable energy system integration, efficient energy conversion technologies, effective process integration, and effective techniques to enable a circular economy framework, and other issues that are important to the population. Economic growth, modernization, and automation are mainly depending on the energy supply. The carbon dioxide emission causes greenhouse effect and environmental degradation which threaten the global environment. Worldwide greenhouse gas emissions are steadily increasing on a global scale, where climate change concerns are becoming increasingly prevalent and wreaking havoc on the people. CO_2 emissions have grown by around 2.7 percent, making them the most dominant emissions. This recent surge in CO_2 emissions is very alarming, especially given that CO_2 levels were nearly steady.

It is obvious that current measures to control these emissions are insufficient and that strong and timely global actions are required to attain this aim and, as a result, to limit the adverse effects of anthropogenic activities on the environment. It is the requirement for long-term development that leads to the integration of cost-effective ways based on interdisciplinary knowledge. Globally, fossil fuels are still used to generate power to a great level, accounting for more than half of all electricity generation, mostly coal, and natural gas. One of the major problems with current fossil fuel energy systems is their low conversion efficiency, which results in a high rate of thermal energy waste.

The renewable energy generation level increases as the energy development, which relies on the reduction of fossil fuel generation. The fossil fuel is taken as a primary source of energy to satisfy the supply of energy demand. This fossil fuel emits greenhouse gases and create hazard to environment and affect the future generation. So, the sustainable energy resource is of great significance to reduce the fossil fuel consumption. The renewable energy resources are free from emission. The renewable energy with smart technology provides an idea for the emission problem and contributes significantly in generating power with less emission of greenhouse gases. Increased energy demand, along with the depletion of fossil fuels, has heightened the

need for rapid development of renewable energy (RE) sources to meet demand. However, the use of renewable energy as a percentage of total energy consumption in many nations is still at a low level. RE is needed for a variety of activities, including lighting, heating, and cooking, and it may originate from a variety of sources, including biomass, solar, wind, and hydropower. The costs of developing various alternative energy sources to meet the energy needs of a certain location are varied. It these challenges that call for researchers to come together and show case they findings with intentions of coming up with energy solutions that will mitigate these growing challenges.

In this year's conferences on Mathematical, Pure and Applied Sciences and Energy and Environment 2023, I am informed that they have attracted some good papers on the above mentioned fields of materials simulation to applications in solar panels and weather simulations. Presenters range from undergraduates, independent researchers to lecturers from both public and private universities with quality work. I am told we have presenters from South Africa and Tanzania.

Keynote Address 2

Professor Kapil Mohan Khanna
Akido College of Engineering (Bahadurgarh, India)

Introduction

Basic science is concerned with the process of discovery of new ideas or theories, of how natural systems such as human cells or plant cells and of gravitational and interstellar bodies etc. functions. The research effort is concerned with how they will use the discovery of the newly acquired knowledge. The objective of the 'basic research' is to answer the 'what' 'how' and 'why'. It is mainly performed at Universities, Academic Institutions, Research laboratories where the main reward is publication of the research in a scientific journal. In fact, general basic research is rather far away or not a part of market setting. The scientific disciplines known as physics, biology, chemistry, and mathematics, are called 'Basic sciences'. They are called basic sciences since they provide a fundamental understanding of natural phenomena and the process by which natural resources are transformed (Stokes, 2011).

Science is involved in all kinds of human activity like cooking, eating, breathing, driving, playing etc. Every activity is a consequence of the advancements in science. Life cannot exist without all this. The impact of Interstellar System on the sustainability of human life needs all kinds of scientific laws, especially the laws discovered by physics and mathematics. Remember that science is a systematic and logical study towards how the universe works. Science is a dynamic subject and it is not based on fixed ideas. What is valid today can change tomorrow with a new discovery. In fact, science can be defined as the systematic study of the nature and behavior of the materials (human being included) and physical universe based on an observation, experiment and measurement and the formulation of their laws to describe these facts. Science is one of the greatest blessing and gift to manifest to mankind. It has played a major role in improving the quality of living of the mankind. Science is universal, omnipresent and omnipotent in every walk of our life. In every inch of our body, science is the protagonist. Basic science increases the knowledge base of a field of research and helps us with knowledge to solve specific problems. There is a theoretical framework from which one can draw to develop resolutions to reveal problems

Applied Science

Applied science is the use of 'scientific method' and knowledge attained via conclusions from basic science to attain practical goals and includes broad range of disciplines such as 'medicine' and 'engineering'.

- ➢'Applied science' is generally contrasted with 'Basic science' whose focus to advance 'scientific theories' and 'laws' that explain and predict natural and other phenomena. (Bunge, 1966)
- What is the difference? Indeed, applied science can usually apply formal science such as 'statistics' and 'probability theory' as in epidemiology is an applied science applying both biological and statistical methods.
- ➢Applied science can also apply social science such as applications of psychology in applied psychology, Criminology and law.
- ➢Applied science is said to be invisible revolution brought about by the application of 'basic science'. (Donnelly, 2009)
- ➢Basically Applied Science refers to using theoretical scientific knowledge for practical applications such as new invention based on existing knowledge or tool.

- An applied scientist conducts scientific analysis with a goal of applying the theoretical findings to real world solution.

➢Applied science or research is closer to market setting and involves a large scale commercial horizon.

➢It leads to preparations for commercials, applications, and exploitations.

➢In general, applied research is protected, confidential and secret in its applications.

➢Applied science typically covers areas related to four basic sciences i.e. Biology, Chemistry, Mathematics and Physics.

➢It can as well deal with some applied scientific disciplines such as biomedical sciences, space sciences etc.

Bridging the gap

➢Basic and applied biology

➢Historically, biology disciplines have experienced mergers (Ross, et al.,2013 (DMM)-Disease Model of Mechanisms for instance, embryology and genetics were once seen as separate Disciplines they had different goals and emphasis.

➢Ultimately, the two fields merged as the goal of embryologists and geneticists aligned and their knowledge became sufficiently overlapping which enabled them to speak the same language.

➢Similarly, mergers have taken place between (i) Cell biology and Neurophysiology and (ii) Evolutionary biology and Developmental biology.

➢Such mergers bridge the gap between basic and applied biology.

➢In fact, 21st century is recognized as the century of great merger of basic and applied biology.

➢The confluence of forces is now accelerating and bridging the gap between basic and applied biology hence the output from an experimental apparatus depends on the theoretical input from mathematical physics and digital electronics.

➢As our understanding of biological process deepens, it will aid the development of rational approaches to disease.

➢For major diseases clinical trials based on our preclinical was used to understand the impact of diseases on mankind.

➢Today we have achieved nanometer resolutions in our investigations our tools have become more powerful and the level of improvement is accelerating.

➢We are now trying to imagine how these tools can be applied to diseases and it is here where the bridging the gap between basic and applied biology will be essential activity.

Bridging the gap between theoretical and applied chemistry.

➢Theoretical chemistry is the branch of chemistry that develops theoretical generalization and concepts of chemical bonding chemical reactions valence the surface of potential energy molecular orbitals orbital interactions and characteristics of molecules via molecular activation (Gordon,1996).

➢Another recent branch of theoretical chemistry is known as computational chemistry which is the branch of chemistry that uses computer simulation to assist in solving chemical problems.

➢It uses methods of theoretical chemistry incorporated into computer programs to calculate the structure and properties of molecules groups of molecules and solids.

➢It is necessary because apart from relatively recent results regarding the hydrogen molecular ion (dihydrogencation) The quantum wavy body problem cannot be solved analytically much less in closed form whereas computational results normally Compliment the information obtained by chemical experiments.

➢It can in some cases predict either to unserved chemical phenomena-a clear method of bridging the gap between theoretical and experimental (or applied) chemistry.

➢It is now Widely used in the design of new drugs and materials. (Smith and Sutcliffe, 1996)

Pure and Applied Mathematics

➢Bridging gap between pure and applied mathematics

➢Pure mathematics focuses on practical fields and helps in innovation and discovery of new ideas.

➢In fact, pure mathematics is any mathematics that has not yet found use or adoption outside of the mathematics community.

➢Applied mathematics focuses on solving problems arising at fields such as economics, finance, biology, physics, and engineering.

➢On the other hand, pure mathematics focuses on solving the problems encountered by other mathematicians.

➢Pure mathematics involves using pure numbers while whereas applied mathematics involves quantities such as numerical values and units of measurements.

➢Pure mathematics refers to algebra number theory, geometry, differential and integral calculus, differential equations of all kinds.

➢Pure mathematics is a sort of fact that may be speculative and imaginary whereas applied mathematics deals with practical problems inspired by other sciences and engineering.

➢Use of differential equations, integrations, Green's, function etc. When applied, problems in engineering such as fracture mechanics, theoretical mechanics, heat transfer are examples of bridging the gap between pure and applied mathematics.

➢Finally, pure mathematics means going deep into math only for the sake of studying and advancing mathematics.

➢Whereas applied mathematics deals with solving experimental physics and engineering problems. (Logan,2013)

Pure and Applied physics

➢Physics

➢It is said that the best physics eliminates complexity by revealing underlying simplicity.

➢Now, this is a very simple way of defining what physics is all about.

➢In reality, physics is a very complex science that requires sufficient, and up-to-date, knowledge of almost all the basic sciences and many aspects of engineering, even the physics can be divided into two simple segments to illuminated contents, one segment is theoretical physics and the other is experimental physics.

- In theoretical physics, there is theoretical framework from which one can draw to develop solutions to real problems.

➢One can say that the mathematics of theoretical physics is mostly modelling, but in reality, it uses ordinary mathematics starting from Quadratic Equations all the way to complex theory of complex variables, Green's functions, operators and second quantification, many body theory to theoretically study of properties of systems in atomic physics, nuclear physics, solid state physics, and so on.

- As such theoretical Physics is thus a branch of physics that employs mathematical models and abstractions of physical objects and systems to rationalize, explain and predict natural phenomena.

Experimental and Theoretical Physics

➢But in experimental physics, one uses experimental tools to probe the natural phenomena and make predictions such that one can bridge the gap between theoretical results and experimental results to decide which theoretical model may be more accurate to describe the newly discovered phenomena. (Joos and Freeman, 2013).

➢Sometimes phenomena is first discovered experimentally and then its theoretical explanation is proposed later and sometimes a phenomenon is proposed theoretically and its explanation or experimental observation is done later.

➢Superconductivity in Raman's effect are two phenomena that fall under this category.

Superconductivity

➢Superconductivity was discovered (Onnes, 1911) when the resistance of mercury was being measured at a very low temperature.

➢At the temperature of $T<4K$, the resistance suddenly disappeared and very large currents (105 A) flowed through the Material.

➢Many theories were proposed to explain the phenomena, but none of the theories were very successful.

➢In between most superconductors were discovered that indicated that superconductors have different transition temperatures different types of coupling between the electrons in the superconducting state and hence successful theory required to bridge the gap between experimental observations and information obtained with the theoretical modeling of coupling between the electrons.

➢First such a theory was proposed very late in 1957 and is called BCS Theory (Bardeen, et. al,1957)

➢Later a lot of theories based on experimental input were proposed using methods of second quantification and many body theories. [14] [Khanna.K.M, Kirui.M.S.K. Indian Journal of pure and applied physics, 40(2002)007] [15] [Khanna.K.M, Superconductivity, Moi University Eldoret KENYA.3 Series No.1(2008)] [16] [Kiboi.D. Chenge, Peter Tanui, Limo.C. Samuel, Kapil.M. Khanna, Electron Hole Superconductivity in Bilayer Graphene Superconductors. SITA, No.2,3, Vol.25(2023)].

➢Thus bridging between information obtained experimentally and the theoretical modelling is necessary for a complete understanding of the phenomena.

Raman Effect

➢Raman effect is the scattering of light from a molecule in which the scattered radiation Modified frequencies that can be more and less than the frequency of the incident radiation.

➢This phenomenon was theoretically proposed first by Adolf Smekal in 1923 [17] [Boris Podolsky and Vladymir Rojansky. On The theory of Smekal Raman Effect in hydrogen like atom, Phys.Rev3491929)1367] ($39.95)

➢Smekal proved theoretically, that the scattered radiation will have frequencies higher and lower than the frequency of the incidental radiations since the number of Scattered photos is very small compared to the total number of incident photons, the intensity of the scattered radiation was small and difficult to detect in those days when the experimental apparatus were crude and not very reliable.

➢It was Professor C.V Raman in India who experimentally discovered this Phenomena in 1928. For this, he got Nobel Prize in Physics 1932

➢The radiation scattered with frequency Less than the incident, radiation is called stroke lines scattered Radiation with frequency more than the incident radiation is called anti stroke lines. [18] [Raman. C. V Indian Journal of Physics, Vol1(1928)]

➢With the improvement of experimental apparatus and discovery of laser radiation, Raman effect is now extensively used in physics and medical diagnostics, especially in the location of ca**ncero**us cells.

➢Experimental studies on Raman effect, and the development of theories on Raman effect are classic examples bridging the gap between Theories and applied physics. [19] [Khanna. K. M and Murei. K. G; Effect of oscillating electric field due to oscillating electric dipole on Raman lines East European Journal of physics.4(2019)47-57] similar example existing nuclear theory, Solid state physics and nuclear astrophysics.

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Conference Abstracts

Expanding the Scope of Computational Alchemy for Efficient Screening of Non-Noble Transition Metal-Doped Pt Catalysts for CO_2 Reduction

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Abstract
Density functional theory (DFT) has been widely used for deriving descriptors in the screening of alloy configuration spaces. However, the computational costs associated with DFT limit its practicality for expansive alloy systems. In recent years, computational alchemy has emerged as a promising alternative for approximating descriptors with reduced computational requirements. By utilizing a single set of reference DFT calculations, computational alchemy enables the efficient screening of random/hypothetical alloy configurations. In this study, we focus on the screening of non-noble transition metal-doped Pt catalysts for CO_2 reduction. We employ computational alchemy to approximate descriptors based on binding energy and explore its efficacy in screening a diverse range of alloy compositions. By thoroughly examining the limitations and challenges of this approach, we provide insights into its applicability for efficient catalyst screening. Our results demonstrate that computational alchemy predictions of adsorbate binding energies closely align with those obtained through DFT calculations, validating the effectiveness of this method for materials screening. Through this research, we extend the scope of computational alchemy beyond DFT, showcasing its potential as a cost-effective tool for screening non-noble transition metal-doped Pt catalysts for CO_2 reduction. This study contributes to the advancement of efficient materials screening techniques, enabling the accelerated development of catalysts for sustainable CO_2 conversion. By expanding the capabilities of computational alchemy, we pave the way for more comprehensive and cost-effective catalyst design strategies.

Keywords: Catalyst, screening, alchemy, CO2 reduction, doping, DFT

Thermodynamic Parameters for Hydrogen Storage in Metal Organic Frameworks

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Abstract
The global energy crisis and the rising demand to decarbonize the planet have escalated research on an alternative clean energy in the changing energy mix. Owing to the abundant availability and natural inexhaustibility of hydrogen in nature, the green hydrogen has turned out to be a promising and an attractive energy carrier in cars and other mobile applications. However, hydrogen production still faces challenges on storage, distribution and usage. Microporous metal-organic frameworks have become the most promising materials for hydrogen storage since they have high surface areas and chemically tunable porous structures. Thus, this study is carried to investigate the theoretically valid equations and thermodynamic

parameters for hydrogen storage in metal organic frameworks. Our calculations revealed that an efficient hydrogen storage metal organic framework should be tuned to high overall entropy above $484\,J.mol^{-1}K^{-1}$ at room temperature, $\Delta G \cong 2000\,J/mol$ and $\Delta H \cong 1500\,J.mol^{-1}K^{-1}$ at $P(T)$ between 40 $bar$to 100 bar.

Tungsten Doped TiO_2 for Organic Dye Removal from Wastewater

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[3] Department of Physics, University of Dar es Salaam, Tanzania.

Abstract 03
Wastewater contains a variety of harmful substances ranging from heavy metal ions, bacteria and organic pollutants. Photocatalytic technique plays a vital role in reduction of toxic impart of organic dyes in industrial wastewater. In regard to this, photocatalytic tungsten doped TiO_2 (W-TiO_2) was prepared by anodization method on a titanium plate substrate. The effect of different tungsten concentration on the photodegradation activity of TiO_2 was studied on crystallinity, surface roughness and charge carrier density by XRD, AFM and electrochemical impedance spectroscopy analysis. It was found that at 5%.wt. W-TiO_2, a more rough film was formed. The increased surface roughness as depicted by the AFM images provided more adsorption sites for the dye hence increased photodegradation rate of 79% was achieved. Annealed samples had high charge separation rate compared to amorphous one and hence high photoactivity.

Keywords: Anodization, W doped TiO_2, Photodegradation, Organic dye removal.

Influence of the Substrate Temperature and Ag Incorporation on the Properties of Reactively DC Co-Sputtered Ag:TiO_2 Thin Films

Hezekiah Buay Sawa[1], Margaret Emanuel Samiji[1], Nuru Ramadhani Mlyuka[1],
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Abstract
This study reports influence of the substrate temperature and Ag incorporation on the structural, morphological, optical transmittance and Hall Effects parameters of Ag doped TiO_2 thin films. Films were deposited on the glass substrates by DC co-sputtering of Ti and Ag targets in the O_2 (g) and Ar (g) atmosphere at different substrate temperatures and Ag sputtering powers. The increase of Ag relative intensity from Glow Discharge Optical Emission Spectroscopy (GDOES) measurement approved increase of the incorporated Ag amount of into TiO_2 film as sputtering power was increased from 0.2 W to 1.5 W. X-ray diffractometer (XRD) confirmed that all films have the polycrystalline structure with dominant peak oriented along (101) plane representing anatase TiO_2 structure. XRD and SEM results showed significant influence of the substrate temperature on the crystal, grain sizes and compactness. Electrical conductivity as

determined from the Hall Effect Measurement System (HMS) was found to increase with increase in substrate temperature. UV-VIS-NIR spectrometer showed that the film transmittance was decreasing with increase in temperature and Ag sputtering powers when temperature was kept constant. The Ag doping showed decrease in bandgap energy from 3.4 eV (undoped film) to about 3.2 eV (doped films). Furthermore, analysis of the atomic force microscopic images showed grain distributions and surface roughness are influenced by the substrate temperature. The good compromise of the electrical conductivity (1.304 $(\Omega cm)^{-1}$) and transmittance (above 62% weighted average with glass) was obtained at substrate temperature of 400 ^{o}C and sputtering powers of 0.2 W and 0.5 W for Ag. From RBS measurement, it was confirmed that 0.5 W sputtering power of Ag target gave a 0.28% concentration. The findings from this work demonstrate potential deposition approach for Ag doped TiO_2 and its wide application as TCO in photovoltaic cells.

Key words: substrate temperature, Ag incorporation, Ag doped TiO_2, reactive co-sputtering

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Influence of WO3 doping on Optical Properties of SnO2 Thin Films Synthesized by Sol-gel Spin Coating Technique

Victor Isahi[1], Christopher Maghanga[1], Mghendi Mwamburi[2], Onesmus Munyati[3],Sylvester Hatwaambo[4], Emmanuel Akoto[1], Wycliffe Isoe[5], Mir Waqas Alam[6]

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Abstract

Metal Oxides have received increasing research interest in recent years due to their applications in the energy and environmental domains. Tin (IV) Oxide (SnO_2) has ardently been investigated for various applications due to its remarkable properties, non-toxicity, and stability. However, its wide bandgap and the tendency for some electrons and holes to recombine have been cited among the limiting factors. This study, therefore, aimed at preparing and optimizing SnO_2 thin films by doping it with varied proportions of Tungsten (VI) Oxide (WO_3) and investigating the effect of WO_3 doping on the optical properties of the films such as absorbance, optical constants (n & k), and band gap. Doping improved the optical absorbance of the films and caused a red shift on the absorption edge of the films decreasing the band gap from 3.82 to 3.03 eV This results showed that doping has a strong influence on the optical properties of Tin (IV) Oxide thin films, providing a tool for improving the film's properties for applications in environmental and energy domains.

Key Words: Sol-gel spin coating Tin (IV) Oxide Doping Optical Properties

Piezo - Photocatalytic Performance of Fe- Doped BaTiO3 Compounds

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Abstract
Persistent organic compounds in industrial effluents and their efficient removal technique have emerged as a crucial problem to waste water treatment plants. Among many proposed methods, photocatalysis stands out as an efficient and sustainable oxidation technology in waste water treatment since it allows complete mineralization of toxins. Further, the development of visible light photocatalysts to address water pollution is essential since visible light constitutes a good fraction of the solar spectrum. Research has suggested many photocatalysts, barium titanate ($BaTiO_3$) being among them. A semiconductor perovskite material, $BaTiO_3$, stands out to be a promising photocatalytic compound. This is because $BaTiO_3$ exhibit inherent chemical activity since it is a ferroelectric material. To enhance its photocatalytic performance under visible light, this study investigated the effect of Fe doping concentration on its bandgap and its photocatalytic performance. The undoped and Fe-doped $BaTiO_3$ films were synthesized through sol gel technique and deposited on glass substrate through spin coating technique. The photocatalytic activity of $BaTiO_3$ films was evaluated through photo degradation of methyl blue aqueous solution. The bandgap reduced from 3.26 eV to 1.59 eV for undoped and 0.5%wt doped samples respectively. Further analysis revealed that 0.5%wt Fe loaded sample had the best photocatalytic performance with degradation constant of 2.37×10^{-3}. Annealing was observed to greatly improve the photocatalytic performance of the samples. These results demonstrate the potential of employing Fe-doped $BaTiO_3$ as a visible light photocatalytic material.

Key words: piezo-photocatalysis, BaTiO3, photodegradation, ferroelectricity

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Mechanical Properties of Al-Mg-Si Alloys (6xxx Series): A DFT-Based Study

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Abstract
Aluminum (Al) and its alloys have a wide range of applications such as in cooking wares, cladding in buildings, and electric cables. This is due to the advantages that they have, which include low density, good thermal and electrical conductivity, and availability. Several studies, mostly experimental, have been done on the mechanical properties of aluminium magnesium silicon alloys (Al-Mg-Si). However, other mechanical properties such as bulk modulus, shear modulus, and Youngs modulus have not been explored extensively. This study investigates the bulk modulus, shear modulus, Youngs modulus, Poisson's ratio, Pugh's ratio, and Vickers hardness of the Al-Mg-Si alloys. The modelling of the structures was done using Al cell as the starting structure, where nine structures of Al-Mg-Si alloys with different percentages of Al, Mg and Si were modelled. Calculations of elastic constants were done using the stress-strain method within the density functional theory as implemented in the *Quantum Espresso* code. The optimum properties obtained in this study were: density of 2.762g/cm^3, bulk modulus of 83.3GPa, Shear modulus of 34.4 GPa, Vickers hardness of 2.79 GPa, Poisson's ratio of 0.413, Pugh's ratio of 5.42, and yield strength of 8.38 GPa. The optimum Si/Mg ratio is found to be 4.5 for most of the mechanical properties. The study successfully established that Si/Mg ratio is a critical factor when dealing with the mechanical properties of the Al-Mg-Si alloys. The alloys at the optimum Si/Mg ratio can be used for industrial applications where the properties are required such as in plane skins and mining equipment.

Key words: Aluminium alloys; Al-Mg-Si alloys; mechanical properties of Al-Mg-Si alloys; Si/Mg ratio on mechanical properties of Al-Mg-Si alloys; aerospace and automotive materials, Density Functional Theory

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Electronic Structure and Dynamical Properties Study of Strontium Doped Barium titanate; Ba1-xSrxTiO3Perovskite; A First Principle Study

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Abstract
Barium strontium titanate $Ba_{1-x}Sr_xTiO_3$ can be prepared using different methods depending on its application since the method used in its preparation influences both its structure and properties. Increase in strontium concentration decreases its band gap which implies that it also changes from an insulator to a semiconductor. This study reports electronic structure and dynamical properties dependence of $BaTiO_3$ on Sr concentration. Density functional theory in the framework of quantum espresso code is here applied to analyze the effect of Sr variation in a supercell of 42 atoms and a cut-off energy of 500 eV. With a concentration of Sr of 0.25 band gap decrease with a value of 40.8% and doping with 0.5 Sr reduces the gap by 0.99%. This shows that Sr doping should not exceed 25% for any meaningful band gap change.

Key Words: Barium, titanate, Dielectrics, perovskites

Bayesian methods in Medical Research: The case of Survival Models

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Abstract
The Bayesian approach has increased in popularity in medical data modeling due to its flexibility in accommodating high-dimensional distributions and incorporation of priors in analysis. Recent developments in computational tools to handle Markov Chain Monte Carlo (MCMC) techniques have made Bayesian analysis even more convenient for researchers. This paper outlines the Bayesian inference for the Weibull survival model with censoring mechanism using simulated and real data. A step-by-step explanation of the Bayesian approach process is presented. The implementation of Bayesian inference is through the conventional WinBUGS and R software. Illustrations are provided to demonstrate the computational power of these tools in medical data modeling.

Keywords: Bayesian methods, Medical data modeling, R, Survival models, WinBUGS.

Development of an Automated Hall Effect Experimentation Method for the Electrical Characterization of Thin Films

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Abstract
There has been drastic growth in the microelectronics industry in the recent past. The performance of these materials is influenced by their structural, electrical, and optical properties among others, depending on their applications. Therefore, the need to conduct measurements of the semiconductor characteristics precisely, quickly, and conveniently cannot be overstated. Some of the desirable features of measurements include usability, accuracy, resolution, repeatability, and consistency which cannot be assured with manually operated systems. This study strived to design and interface an automated computer-aided four-point probe test equipment that characterizes materials to determine their electrical properties. A four-point probe head, an electromagnet, NI Keithley model 6220 Precision current source, model 7001 switch, model 2182A Nano voltmeter, and model 7065 Hall Effect card instruments were interfaced with the NI LabVIEW program running in a computer through a GPIB hub to a PC USB for its full control. The four-probe head was utilized to probe the samples with a square symmetry that was adopted for the measurement of the semiconductor properties. Reliability tests were conducted on a standard P-type Germanium sample. The collected data was within 0.32% of the expected results. This work forms a basis for automating similar systems that were inherently designed to be operated manually.

Structure and properties of superconducting Magic Angle Twisted Bilayer Graphene

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Abstract
Magic-Angle twisted bilayer graphene and trilayer graphene exhibit superconductivity that even survives under strong magnetic field. This means there exists strong correlations between the electrons that constitute Cooper whose existence is necessary to describe the superconducting state. Thus misaligned graphene layers are used to investigate strongly correlated Physics in which the interaction between the electrons, electrons and phonons, lead to novel phenomena. The role of coulomb interaction between the electrons, and between the electrons and holes, that may travel independently in two separate layers separated by a dielectric is an important area of investigation. Calculations using these ideas are done to determine the specific heat, C_v, entropy, S, and transition temperature, T_c, and are compared with the experimental results about graphene superconductors. Graphene is a correlated insulator which becomes a superconductor by adding a few extra charge carriers (electrons, or holes or both) to the insulator state by applying a small electric field. This means that the charge carrier density is important in realizing the superconducting state.

Key words: Twisted Bilayer Graphene, Strong correlations, Cooper pairs, Coulomb interaction, Charge carrier density