THE ETHIOPIAN PHYSICAL SOCIETY (EPS)

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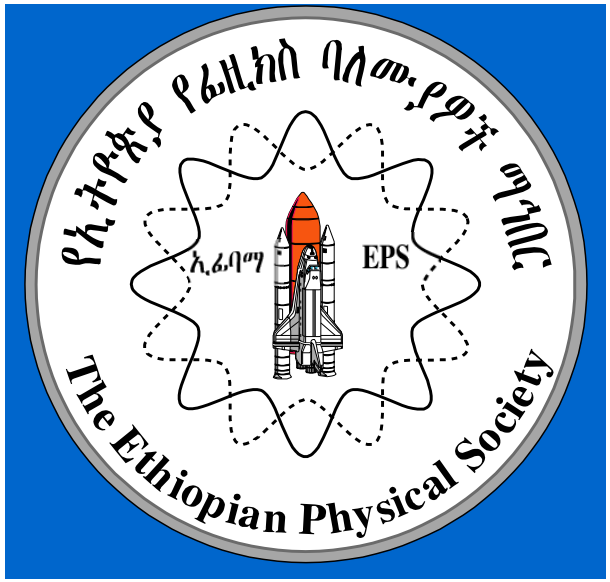
THE ETHIOPIAN PHYSICAL SOCIETY (EPS)

BOOK OF ABSTRACTS

TWELVETH NATIONAL CONFERENCE



February 23 & 24, 2018

VENUE:

College of Natural and Computational Sciences

Addis Ababa, Ethiopia

CONTACT ADDRESS:

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Foreword

The Ethiopian Physical Society (EPS) will held at the 12th Annual National Conference in the premises of the College of Natural and Computational Science of the Addis Ababa University on February 23-24, 2017.

It is expected that this year event will be a great success to our Society thanks to the active participation of its members as well as the financial and material support of various organizations and institutions. On behalf of its members, the executive members of EPS would like to express their gratitude to all sponsors which provided the necessary support to organize the current Conference. In particular, our thanks goes to: General Electric, the Ministry of Science and Technology, the Department of Physics of AAU, Entoto Observatory and Research Center, BGI Brewery, Meta Abo Brewery, and Walia Brewery, as well as the Ethiopian Physical Society – North America and the Gholap Foundation for providing financial support for female students' awards.

As usual, the willingness and interest of our members to present their research findings is highly motivating. About twenty research papers, covering different areas of physics, are expected to be presented during the Conference. The Executive Committee members would like to extend its appreciations to all paper contributors.

Lastly, the Executive Committee of EPS wishes all the participants a fruitful and enjoyable Conference. We would like to extend our invitation to all participants to make your utmost contribution for the successful conclusion the Conference.

Dr. Deribie Hirpo
Secretary

Dr. Chernet Amente
President of EPS

Dr. Gelana Amente
Vice President

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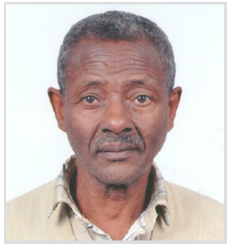

Dr. Mulugeta Bekele
Public Relations

Dr. Mesfin Asfaw
Editor-in-Chief

The Effect of Temperature on Optical Properties of ZnO@ Ag Core - Shell Spherical Nanostructure in the Host Matrix of MgF_2

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Abstract

In this study we investigated the effect of temperature on the optical properties of ZnO@Ag core - shell nanostructure embedded in the medium of magnesium difloride (MgF_2) which have dielectrics constant 1.93. Temperature dependence of the plasmon resonance is important issue because of recent applications of core - shell NPs for heat treating of cancer and the computer chips, communication device, signal processing, medical and biological applications and different optical applications depend on it. Polarizability, refraction index, optical absorbance and transmittance, absorption and scattering cross section of ZnO@Ag core – shell spherical nanostructure is studied at different temperature with the rage of 200 K and by varying radius of quantum dot of ZnO and/or thickness of Ag from Drude model, Lorentz model and Mie theory kept filling factor $f = 10^{-3}$. Absorbance, scattering cross section, absorption cross section and other optical properties are minimum in visible region and maximum in UV region.

Solar Activity on Ethiopia Ionosphere by Using Ground Based GPS Data Located at Adama, Ethiopia

Amensisa Negasa

Abstract

Ionization is the procedure of making absolutely or adversely charged particles or atoms by including or striping one or more electrons. For the case of Earths atmosphere Ionization can occur because of solar radiation. On this paper we shows affects of solar activity on Ethiopia Ionosphere by using Adama, Ethiopia ground based GPS data. We collated this data by using ground based GPS receiver located at Adama (8.5^0 N and 39.2^0 E) have been analyzed to study the temporal variations of the ionosphere in the region. We have investigated the effects of sunspot on the characteristics of the total electron content (TEC) values. According to our data the observed TEC values are minimum at pre-down throughout the year, followed by a steep increase in its value in the intervals 1000UT-1400UT. This may be due to the variation of the strength of solar radiation that reaches the atmosphere. The observed TEC values are correlated with sunspot numbers as there are more radiation (X-ray and UV) from the Sun during large number of sunspots.

Friday - February 23, 2018

8:30 – 9:30 AM	**Conference Registration**	
9:15 AM	Opening Remarks by the Guest	Guest
9:30 AM	Welcoming Remarks by EPS President	Chernet Amente
Morning Session I – Chairman: Gelana Amente		
9:50 AM	STEM: Imperatives in Our Education System: View Point	Tilahun Tesfaye
10:10 AM	Physics Education in Ethiopia	Mekbib Alemu
10:30 AM	Investigation of the Relationship Between College Physics Curriculum and Primary School Physics Curriculum	Alemu Kebede
10:50 – 11:15 AM	Tea Break	
Morning Session II – Chairman: Lemi Demeyu		
11:15 AM	General Electric - Missions and Objectives	Tesfaye Kidane
11:30 AM	Phase Diagram of π-Conjugated Polymer Solution: Upper Critical Solution Temperature Behavior	Jung Yong Kim
11:45 PM	Heavy Ion Induced Nuclear Reaction Dynamics at Low Incident Energies	M. Afzal Ansari
12:00 – 2:00 PM	Lunch Break	
Afternoon Session I – Chairman: Getachew —— (HU)		
2:00 PM	Spin-Dependent Transport in Diluted Magnetic Semiconductor: ZnSe/Mn Doped Hetrostructure (Quantum Wire)	Genene Shiferaw
2:15 PM	Improved Surface Adhesion of $KY_3F_{10}:Ho^{3+}$ Thin Films at Elevated Deposition Temperature	Nebiyu Gmechu
2:30 PM	Elemental Characterization of Indigenous Food Cereal, Hordeum volgare, using Neutron Activation Analysis Technique and Gamma Ray Spectrometry	Getaneh Ayele
2:45 PM	Multi Elemental Analysis of Indigenous Food Spices in Southern Ethiopia using INAA Technique	Tamene H.M.
3:00 – 3:30 PM	Tea Break	
3:30 – 4:30 PM: **Afternoon Session II (Contd. … on Page 4)**		

Afternoon Session II – Chairman: Sisay Shewamare		
3:30 PM	**Density Functional Theory Fundamentals and Practical Applications**	Gamachis Sakata
3:45 PM	Density Functional Theory Study on the Effect of CO_2 Contamination in Rechargeable Na-Air Batteries	Natei Ermais
4:00 PM	Computational Study of Formation and Structural Growth of a Layer of Hafenen on Ir(111) Surface	Kumneger Tadele
4:15 PM	Dielectric and Relaxor Ferroelectric Properties of $SR_4CALATI_3NB_7O_{30}$ Tetragonal Tungsten Bronze Ceramics	Gebru Tadesse
4:30 PM - End of first day of the Conference		
Morning Session I – Chairman: Getahun Kitile		
9:15 AM	Diagnostic Assessment of Random and Incoherent Students' Responses of Core Physics Concepts Using Concentration Analysis	Bekele Gashe
9:30 AM	Investigation of Chlorophyll and Beta-Carotenoids in edible oils by absorption & Fluorescence Spectroscopy	Tewodros Taye
9:45 AM	Concentration, Wavelength & Temperature Dependent Refractive Index of Sugar Solutions & Methods of Determination Contents of Sugar in Soft Drink Beverages	Abebe Belay
10:00 AM	Application of Image Processing Technique to Study Malaria Parasites in Blood	Tensael Tarekegn
10:15 – 10:45 AM	Tea Break	
Morning Session II – Chairman: Tesgera Bedassa		
10:45 AM	INDOSAW - Industrial (Scientific Equipments) Products	Ajay Sagar
11:05 AM	Geospace Monitoring Research: In Equatorial Africa	Ephrem Tesfaye
11:20 AM	Solar Activity on Ethiopia Ionosphere by Using Ground Based GPS Data Located at Adama, Ethiopia	Amensisa Negasa
11:35 AM	The Effect of Temperature on Optical Properties of ZnO@Ag Core-Shell Spherical Nanostructure in the Host Matrix of MgF_2	Gashaw Beyene
11:50 AM – 2:00 PM	Lunch Break	
2:00 PM – 3:00 PM	**Business Session – Chairman:** Deribie Hirpo	
• EPS annual activity and audit report • Regular annual meeting of EPS's members		
6:30 PM	Reception - Closing Session	
End of the Conference		

Geospace Monitoring Research: In Equatorial Africa

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Abstract

This paper investigates how the geomagnetic storm energize the ring current during storm period in July Nov 2013 over geomagnetic equator. The ring current has been determined from Dst value that was computed from ground magnetometer data during an intense geomagnetic storm time over equatorial MAGDAS stations. For a distance 4 times Earth radii the energy content of ring-current was estimated based on experimental observation. In this study around four geomagnetic equator stations had been used. In ala storm period around 9 UT is a time of storm main phase, large amount ring-current and large amount of injected geomagnetic energy were observed over Addis Ababa. The study also showed that as their have reversal relationship and around 3 hrs of interval between Langkawi and Addis Ababa observations. Langkawi attains its main geomagnetic storm while Addis Ababa was in nearly SSC around 06 UT. And around 10 UT Langkawi is nearly in SSC phase, while Addis Ababa was in depression of its storm main phase. On storm time 25 July, 2013 an intense storm at 06 UT had been observed at Langkawi station with strength around -100 nT which lasts around half an hour. After nearly 3 hours interval from geomagnetic storm signature over Langkawi a moderate storm over Addis Ababa happened at 08 UT and its main storm lasts for around 3 hours. On storm 29 July 2013 at 9 UT an intense geomagnetic storm around -55 nT strength with around 8.5 KeV energy content was injected into ring-current of 4 MA as it was observed from Addis Ababa station. The result also shows as around -65 nT geomagnetic storm main phase, at 10 UT around 9×10^{20} (KeV) energy was injected to develop 4.5 MA amount of ring current flowing. After 2 hrs interval from Addis Ababa, relatively less intense storm happened over Abidjan. Relatively before 4 hrs of interval from Addis Ababa over Davao, around -70 nT intense geomagnetic storm, around 4.7 MA ring current flow and 10×10^{20} (KeV) energy content were observed. On 10 August, geomagnetic storm at 06 UT large amount of energy content of 16×10^{20} (KeV) and 12×10^{20} (KeV) were injected into ring current over LKW and TIR respectively. And after 3 hrs interval of this observation 8×10^{20} (KeV) energy was injected into ring currents over Addis Ababa. The study also showed that as their have reversal relationship and around 3 hrs of interval between Langkawi and Addis Abab observations. Langkawi attains its main geomagnetic storm while Addis Ababa was in nearly SSC around 06 UT. And around 10 UT Langkawi is nearly in SSC phase, while Addis Ababa was in depression of its storm main phase. And the effect of main storm phase has 3 hours interval one with another. In all storms it has been found that around 9 UT, it is a time of storm main phase, large amount ring-current and large amount of injected geomagnetic energy content were observed over Addis Ababa.

For modeling of Equatorial ionosphere using NeQuick model. NeQuick is a three-dimensional and time-dependent ionospheric electron density model developed at Aeronomy and Radiopropagation Laboratory (ARPL), ITCP and IGAM, University of Graz. It is a quick-run model specifically designed for transionospheric propagation applications and it allows to calculate the electron density at any given location in the ionosphere and also the Total Electron Content (TEC) any ground station to satellite ray-path by means of numerical integration. NeQuick was originally developed to use the 12-months-running mean R12 or monthly averaged solar flux F10.7 index of solar activity.

To use the NeQuick model for real-time applications such as a Galileo Satellite ionospheric correction model, the monthly averaged solar flux F10.7 index should be replaced by a daily input parameter to take the daily variation of the solar activity and the user's local geomagnetic conditions into account. This daily NeQuick input parameter is the so-called effective ionization level (Az). In this research I develop series algorithms that defines slant Total Electron Content (sTEC) as function of Az which is monotonic. Then once is defined as a function of Az which is monotonic (sTECmod(Az)), the optimum ionization level is determined by comparing model slant TEC with GPS slant TEC in the least square sense.

The correlation of reconstructed slant TEC with GPS slant TEC has been used to evaluate the performance of the reconstruction technique. It has been found that the model fits the experimental observation with the correlation of 0.81, but this is not sufficiently high as compared to similar work in other regions. The physical consistency of the reconstruction technique has also been verified using the diurnal distribution of foF2. It has been found that foF2 attains its maximum during noon time and over ±20 degree geomagnetic latitude (equatorial anomaly region) as expected from theoretical argument. Profiles of electron density derived from the model show two peaks namely E and F regions during the day time and only F layer during night as expected from theoretical analysis.

Keywords: *MAGDAS, Magnetic Data Acquisition System; Dst, Disturbed storm time; critical frequency of F2 layer of the ionosphere (foF2)*

Application of Image Processing Technique to Study Malaria Parasites in Blood

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Abstract

Malaria is a mosquito borne infectious disease of humans and other animals caused by protozoan parasitic of the plasmodium. The most serious and virulent forms of the disease are caused by P. falciparum which contributes to the majority of deaths associated with the disease. Commonly, the disease is transmitted via a bite from an infected female anopheles mosquito, which introduces the organisms from its saliva into a person's circulatory systems. The malaria diagnosis is normally accomplished by visual microscopy which is time consuming and offers low accuracy because of the operator's tiredness and lack of profession in job. To overcome of this liability, we designed an automatic system. The automatic diagnostic process reduces the diagnostic time and also, it can be worked as a second opinion for pathologists and may be useful in malaria screening. The aim of this research is to count the red blood cells that are infected by malarial parasites using digital image processing implementation. As there were the possibilities of other artifacts in the smear blood samples, only RBCs need to be segmented. The artifacts other than RBCs were removed from the image. The resulting image was consisted of only extracted RBCs and used to estimate parasitisimia. Parasitemia was determined as the ratio of the number of infected erythrocytes to the total number of erythrocytes in an image. In this research work, a total of 15 patients' clinical data plasmodium parasite infected blood smears were considered and investigated by using image processing. Based on the developed morphological based code, it was found that, the parasite infected malaria disease can be detected with an accuracy 99.84% sensitivity 99.73% specivity 99.92% based on selected dependent variables.

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STEM: Imperatives in Our Education System: View Point

Tilahun Tesfaye
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Abstract

Practices; trends and outcome of physics education in the Ethiopian school system are examined. National assessments by the ministry of education consistently report that students' performance is unacceptably low in physics and mathematics. Stake holder are complaining on the competencies of the products of the education system at various levels. Should we, in the physics teaching, pause and reflect on what we have been doing decades after decades and years after years? or should we carry on business as usual? In this presentation data on performance assessments are presented along with observations to substantiate the case in point. It is argued that physics teaching practices, in our school system, are problem laden and are not up to the satisfaction of stakeholders including physics teachers themselves. The genesis and universal uses of STEM (Science, Technology, Engineering, and Mathematics) education are highlighted. It is recommended that the existing STEM education activities be scaled up and be embraced by the education system as a whole so as to effect better achievement of learners in their physics lessons and creating scientifically literate society in the long term.

Concentration, Wavelength and Temperature Dependent Refractive Index of Sugar Solutions and Methods of Determination Contents of Sugar in Soft Drink Beverages

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Abstract

The concentration, wavelength and temperature dependent refractive index of sugar solution has been investigated. The refractive index of sugar solutions (5%- 50%) obtained using Red Diode Laser, Green Diode Laser and He-Ne Laser light were found to be in the range of (1.3357 - 1.4117), (1.3467-1.4272) and (1.3380- 1.4140), respectively. The refractive index has linear relationship with the concentration of sugar solution. Mathematical expressions were also derived for the wavelength dependent refractive index of sugar solution by fitting Cauchy's equation to the experimental data using non-linear curve at the minimum discrepancy. The empirical expression of temperature dependent of refractive index of the sugar solution was determined; and the result indicates that, as the temperature increases the refractive index of the solutions decrease The method was also applied to determine the sugar contents in soft drink beverages (Pepsi, Coca, 7up, Sprite, Fanta and Mirinda). The results in g/100ml are: (10.48 ± 0.001), (10.42 ± 0.001), (10.42 ± 0.001), (6.79 ± 0.002), (7.03 ± 0.001) and (9.89 ± 0.002), respectively. The techniques are simple, fast and inexpensive.

Key words:-Laser light, refractive index, temperature, sugar solution and soft drinks

Diagnostic Assessment of Random and Incoherent Students' Responses of Core Physics Concepts using Concentration Analysis

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Abstract

University science students' responses of core physics concepts- energy and momentum-were investigated as they are fundamental and crosscutting concepts in physics. A standardized Energy and Momentum Conceptual Survey (EMCS) test was used to collect quantitative data from 108 first year science students enrolled in a university in Ethiopia. Concentration analysis was used to analyze the students' responses in terms of concentration score, concentration factor and concentration deviation. A one-sample t-test was conducted to evaluate the difference between the average concentration score and the hypothetical random score and showed that there was no statistically significant difference ($t = 0.33$, $p = 0.74$) between the average concentration score and the hypothetical random response score. A paired-samples t-test was conducted to evaluate the difference between the concentrations of students' responses to the scientific conceptions and misconceptions and showed that there was no statistically significant difference ($t = 1.25$, $p = 0.22$) between the two concentrations. The results showed that newly enrolled university science students have low, random and inconsistent conceptual knowledge of core physics concepts. It is recommended that science teachers need to diagnose their students' responses using concentration analysis before commencing classroom instruction and use concepts learning strategies to significantly develop their students conceptual understanding.

Key words: concentration analysis, core physics, diagnostic assessment, misconception, scientific conception

Physics Education in Ethiopia

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Abstract

Both national examination results and many diagnostic test results revealed that science education in general and physics education in particular at a crises conditions. This paper aspires to chart the landscape of physics education in order to categorize problematic areas of Ethiopian Physics Education to direct the research effort in the area. The framework of the analysis here is the quadruplet assemblage interacting elements of the Physics Curriculum, the physics teacher, students learning physics, and the classroom/ school context. After describing the four corners of the quadriporate, observed problems in the current research in the area will be presented. Some of the major shortcomings observed in the current data of research in physics education are the enormous learning gaps in comparison with international picture, the chronically pervasive positivist transmission approach to physics instruction, and the dual stage gap between students' level of readiness and the intended curriculum, and the intended curriculum and implemented one. Finally, recommendations to intensify research effort at all level and refocusing of physics education on socially desired and scientifically prescribed goals of physics teaching by all practitioners were forwarded.

Investigation of the Relationship Between College Physics Curriculum and Primary School Physics Curriculum

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Abstract

The purpose of this study was to investigating the relationship between college physics curriculum and primary School physics Curriculum in Oromia region. The researcher analyzed different documents like college physics courses curriculum guide, college physics courses (modules), college physics laboratory manual, primary school physics syllabus, grade 7and 8 physics text books, and primary school science kit manual. In addition, the study included 34 school physics teachers and natural science department heads working in Shakiso and Adola woreda. And also 8 Adola and Bule Hora Teacher Education Colleges' physics teachers and natural science stream heads were involved in the study. Learning Objectives, contents and all practical activities were analyzed in the documents mentioned. Data relevant to the study were collected using closed ended and open ended questionnaires from college and school physics teachers and interview with school physics teachers. Quantitative and qualitative data analysis approaches were employed. The results of the study show that, the learning objectives stated in the college physics courses syllabus and school physics syllabus give less emphasis for performing scientific process and skills and for developing scientific attitudes and values. Most contents of primary school physics were found in the college physics courses except dimensional expression, electric motor and color code resistor. In document analysis 72.72% of practical activities in school physics text books and 62.5% of practical activities in college physics courses which needs laboratory work (experiment) were not contained in college physics laboratory courses. Based on the result of the study the following conclusion can be drawn: behavioral objectives stated in both curricula do not promote physics education, as well as practical activities in college physics courses and laboratory manual were not prepared in line with primary school physics text books.

***Key words**: primary school physics, college physics courses, learning competence, behavioral objectives*

Investigation of Chlorophyll and Beta-Carotenoids in edible oils by absorption and Fluorescence Spectroscopy

Tewodros Taye and A. V. Gholap

Abstract

In this paper we report the investigation of the absorption spectra, excitation and fluorescence spectra of eight edible oils selected from different countries. Eight samples of oils were purchased from the super markets and included 2 from Spain (olive and extra -virgin olive), 3 from Italy (olive and extra-virgin olive), 1 from Egypt (sunflower) and 2 from Ethiopia (soya bean and Niger seed). To observe the absorption and excitation spectra each sample was diluted by n-hexane (1% v/v) and placed in 10 mm quartz cuvette in Perkin Elmer UV-VIS-Near IR spectrometer Lambeda 19. Spectra was observed in the range of wavelengths 350 nm to 750 nm. Absorption peaks at 410 nm, 414 nm, 470 nm 483 nm, 660 nm, 671 nm were observed corresponding to Chlorophyll A, Beta –Carotenoids and Chlorophyll B, respectively. Fluoromax-4 spectro-fluorometer was used to excite the samples in the range of 360 nm to 420 nm in steps of 10 nm. The fluroscence spectra showed maximum peaks at 467 nm and at 671 nm. Most of the samples showed strong maxima at 671 nm, that corresponds to Chlorophyll A. However, it is worthwhile to note that Sunflower oil indicated smaller peak than other samples containing chlorophyll A which shows that the concentration of Chlorophyll A in the oil is lower than the other oil samples. Moreover, Soya Bean oil had no chlorophyll content.

Key words: Edible oils, UV-VIS spectroscopy, fluorescence spectroscopy, chlorophyll and beta-carotenoids

Dielectric and Relaxor Ferroelectric Properties of $SR_4CALATI_3NB_7O_{30}$ Tetragonal Tungsten Bronze Ceramics

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Abstract

Relaxor ferroelectrics are disordered crystals possessing peculiar structures and properties where at high temperature they exist in a non polar paraelectric phase, which is similar in many respects to the paraelectric phase of normal ferroelectrics. Relaxor ferroelectric $Sr_4CaLaTi_3Nb_7O_{30}$ ceramics were prepared by using the conventional solid state reaction technique. Dielectric property and ferroelectric transition were studied in detail over a broad temperature range. X-ray diffraction analysis revealed that the $Sr_4CaLaTi_3Nb_7O_{30}$ ceramics crystallizes in the tetragonal tungsten bronze structure with space group P4bm. The dielectric studies confirmed two relaxation regions due to the formation of the polar nanoregions below the deviation temperature ~ 405 K. Relaxations I and II were attributed possibly due to the relaxational contributions from dipole reversal of polar nanoregions and fluctuation of polar nanoregion boundaries, respectively. The order of the phase transition of our sample confirms first order phase transition with displacive type of ferroelectric transition. A maximum dielectric constant of 1177 was found at a measuring frequency of 500 Hz. Room temperatures polarization-electric field (P-E) hysteresis loops were assessed and a remnant polarization of 0.65 $\mu C/cm^2$ with a coercive field of 3.33 kV/cm was observed under an applied electric field of 58 kV/cm. The $Sr_4CaLaTi_3Nb_7O_{30}$ ceramics exhibited a prominent dielectric and ferroelectric performance which indicates the potential application of this material in various electronic and energy storage devices.

Heavy Ion Induced Nuclear Reaction Dynamics at Low Incident Energies

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Abstract

The study of the heavy-ion induced nuclear reaction dynamics has been the topic of renewed interest at energies just above the Coulomb barrier and below 8 MeV/ nucleon. The complete and incomplete fusion processes are the two dominant reaction modes in this energy region. In case of complete fusion, the entire projectile amalgamates with the target nucleus and leads to the formation of an equilibrated compound system. On the other hand, in case of incomplete fusion, the projectile may break-up into two fragments near the target nuclear field. Only one of the fragments fuses with the target while remnant moves as the spectator in forward direction with approximately the beam velocity. The dependence of incomplete fusion with various entrance channel parameters like projectile energy, input angular momentum, mass-asymmetry, Coulomb factor (Z_PZ_T) and projectile structure explored in terms of projectile α-Q-value etc could not be established explicitly, which needs more investigation to be unfolded. Non availability of any theoretical models to explain the experimental incomplete fusion data satisfactorily below 8 MeV/nucleon energies makes it still a dilemma. In order to have the better insight into the incomplete fusion study, several experiments based on excitation function (EF), forward recoil range distribution (FRRD) spin distribution and angular distribution measurements have been carried out by using the Pelletron facilities of Inter University Accelerator Centre (IUAC), New Delhi and/or Cyclotron facilities of Variable Energy Cyclotron Centre (VECC), Kolkata, India. Stacked foil activation technique was employed in the above mentioned OFF-Beam and In-Beam measurement techniques. The incomplete fusion process is found to contribute significantly along with complete fusion from the analysis of extracted data at energies 4-8 MeV/nucleon. Different reaction products are also differentiated on the basis of linear momentum transfer from the projectile to the target nucleus. The spin distributions of incomplete fusion products are observed to be distinctly different as that for complete fusion products. The estimated incomplete fusion fraction is observed to be increased with increasing the projectile energy. The projectile structure affects strongly the incomplete fusion which is explored in terms of projectile α-Q -value. Morgenstern's mass-asymmetry and Coulomb factor (Z_PZ_T) effect is observed to be somehow projectile structure dependent.

Phase Diagram of π-Conjugated Polymer Solution: Upper-Critical Solution Temperature (UCST) Behavior

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Abstract

Using thermo–optical analyzer (TOA), the phase separation points for the regioregular poly (3-hexyl thiophene) (rr–P3HT) in 1,2-dichlorobenzene (DCB) solution were measured. The binary rr–P3HT/DCB system shows a conventional upper critical solution temperature (UCST) behavior, which could be described by the Flory–Huggins (F–H) model. Interestingly, it was found that the rr –P3HT/DCB solution shows a partially ordered aggregation even in the one phase state, namely, before phase separation, which was determined by X–ray diffraction (XRD) method.

Computational Study of Formation and Structural Growth of a Layer of Hafenen on Ir(111) Surface

Kumneger Tadele [a,b] , Qinfang Zhang [a, *]

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Abstract

A recent report claims the successful synthesis of two-dimensional (2D) layer honeycomb structure of Hf on Ir(111) substrate. Nonetheless, theoretical discussion on the formation, structural growth and interaction mechanisms of hafenen layer are yet to be adequately addressed. With the purpose of filling this gap, we have investigated the structures and stability of 2D Hf clusters on Ir(111) substrate as the initial stage of hafenen growth using first principles density functional theory (DFT) with the generalized gradient approximation. The study starts with a thorough investigation of adsorption of Hf adatom on the surface of Ir(111). Hexagonal close-packed (hcp) hollow is found to be energetically favorable site for the adsorbent, irrespective of number of adsorbents. The study also reveals the Ir supported 2D Hf clusters of N hexagonal rings prefer a nearly flat honeycomb structure, with exception of N = 1 for which a distorted triangle-like structure is found to be more stable. Neither adsorbed Hf adatom/s nor 2D hafnene layer on Ir(111) surface, unlike to that of free-standing hafenen layer, exhibit magnetic property mainly due to strong hybridization with the Ir(111) surface. The present calculation is supposed to deliver a solid theoretical ground for interpretation and discussion of experimental features of various physical properties and structural growth of hafenen on Ir(111) surface.

Density Functional Theory Study on the Effect of CO_2 Contamination in Rechargeable Na-Air Batteries

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Abstract

The ever increasing demand for sustainable, low carbon emission energy in today's society requires that we develop electrochemical energy storage systems that will exceed those of current technologies. Metal–air batteries (Li-, Na-, and Zn-O_2 batteries) have become promising candidates for modern energy storage due to their high theoretical energy density in comparison to other storage devices. The low cost, low overpotential and abundance of Na compared with Li makes Na–air batteries more efficient in terms of battery lifetime. Here, we apply density functional theory (DFT) calculations to study the effect of CO_2 poisoning on growth/ depletion mechanisms at the steps of stable (001) NaO_2 and (1$\bar{1}$00) Na_2O_2 surfaces, the main discharge products at the cathode of rechargeable non-aqueous Na-air batteries. Adsorption energies of CO_2 at various nucleation sites for both surfaces were determined and their corresponding binding energies show that CO_2 adsorbs strongly at various sites of the surfaces, it would preferentially bind at the left terrace (C) (-1.359 eV) and back step valley (E') (-3.831 eV) sites of (001) NaO_2 and (1$\bar{1}$00) Na_2O_2 surfaces, respectively. We also investigate the reaction mechanisms with and without CO_2 on stepped surfaces of the NaO_2 (001) and Na_2O_2 (1$\bar{1}$00) systems, showing low overpotentials for reaction mechanisms of NaO_2 without CO_2 (η_{dis} = 0. 18 V and η_{cha} = 0.14 V) and high equilibrium potential (U_o=2.57 V), whereas the overpotentials with the presence of CO_2 are found to be prohibitively high (η_{dis} = 0.31 V and η_{cha} = 0.22 V) with relatively low equilibrium potential (U_o = 2.45 V). However, these initial results of CO_2 contamination on (1$\bar{1}$00) Na_2O_2 surface revealed that it slightly increases a charge overvoltage from 0.68 V to 0.74 V, whereas the discharging overvoltage decreases from 0.70 V to 0.64 V. Moreover, the equilibrium potential with the presence of CO_2 is found to be U_o = 2.07 V, which is considerable low relative to the pure surface (2.37 V). In general, the DFT calculations show that in both cases, with and without CO_2, the cells that discharge with NaO_2 exhibit low overpotentials while those that discharge with Na_2O_2 exhibit higher over potential. The reaction processes are strongly influenced by CO_2 contamination, and exhibit increased overvoltages and decreased the efficiencies of the battery.

Key words: NaO_2, Na_2O_2, Na-O_2 batteries, DFT, CO_2 poisoning, Overpotential

Spin-Dependent Transport in Diluted Magnetic Semiconductor: ZnSe/Mn Doped Hetrostructure (Quantum Wire)

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Abstract

Diluted magnetic semiconductors (DMS) are the most promising material in the recent time for spintronic devices. In this work we study the properties and structure of this material specially group II-VI and III-V ferromagnetic DMS which have zinc-blende structure. In addition to this we also deal with the quantum transport in low dimensional semiconductor structures such as quantum wires. As consequence of confinement in two directions, the hole states in a quantum wire are known to be mixtures of heavy- and light-hole components. Due to a strong *sp-d* exchange interaction in diluted magnetic semiconductors, the relative contribution of these components is strongly affected by an external magnetic field, a feature that is absent in nonmagnetic quantum wires. By considering electrons with spin tunneling through DMS/S with a single or double paramagnetic layers we determine the spin- dependent bidirectional group delay(phase time). Spin-polarized transport properties have been investigated in diluted magnetic semiconductor/ semiconductor quantum wires. We stress the effects introduced by the structural configuration and geometric parameters as well as the external magnetic field. It is found that the spin up component of the conductance can be considerably suppressed when the magnetic field is large enough and thus nearly 100% spin polarization can be obtained in such kind of quantum wire. Moreover, one can effectively modulate the spin-dependent conductance in the quantum wire structure by varying the geometric parameters and Fermi energy.

Keywords: DMS, Spin transport, quantum wire, spin dependent

Improved Surface Adhesion of $KY_3F_{10}:Ho^{3+}$ Thin Films at Elevated Deposition Temperature

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Abstract

Thin films have a large role in the current and future industrial technology because of their potential uses as wear-resistant and hard coatings for various applications. Films with low adhesion strength provide little or no wear protection since an applied load could easily remove the coatings. Therefore, films must adhere strongly to their substrates to be useful. $KY_3F_{10}:Ho^{3+}$ *thin films were deposited by pulsed-laser deposition method using Nd-YAG laser (wavelength 266 nm, pulse duration 9.3 ns, repetition rate 10 Hz, and laser fluence 1.2 J/cm*^{2}*, on (100) silicon substrate. At constant target to substrate distance and laser energy, the influence of substrate temperature on the surface adhesion between the substrate and the films was qualitatively analyzed for both argon and oxygen as background gases. The discussion is made in terms of mechanical interlocking, physical bonding and chemical bonding. A method of scratch test was used to qualitatively test the adhesion of the films to substrates. Improved surface adhesion and photoluminescence properties were observed at higher deposition temperature.*

Key words: Characterization, pulsed laser deposition, thin films, surface adhesion

Density Functional Theory Fundamentals and Practical Applications

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Abstract

Density Functional Theory (DFT) is a ground state Ab Initio computational quantum mechanical methods used to investigate the ground-state molecular energy, wave function, and other molecular electronic properties of atoms, molecules, crystals, surfaces, and their interactions based on the ground-state electron probability density, a function of only three variables. Herein with, we have two specific objectives: (1) to introduce DFT in a very brief, consistent and understandable way to emerging quantum computational researchers and even to novice in this field; and (2) to show some practical applications that makes this paper soundable. Furthermore, available DFT codes for free of charge such as GPAW and Quantum ESPRESSO are also highlighted and implemented to calculate benchmark electronic properties such as cutoff energy, lattice parameter, k.points, density of state and band structures. Using Nudged Elastic Band method (NEB), we also showed advanced DFT calculations.

Key words: DFT, GPAW, ESPRESSO, Electronic properties

Multi Elemental Analysis of Indigenous Food Spices in Southern Ethiopia using INAA Technique

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Abstract

The objective of this study is a quantitative and qualitative analysis of essential and trace elements of four indigenous Ethiopian spices and herbs using instrumental neutron activation analysis (INAA) technique. Results obtained for 16 elements: Major elements; Mg, Cl, and K; Minor elements; Na, Fe, and Mn, Zn, Br. While Al, V, Sm, Sc, La, Ba, Eu, Rb were found in traces. The spices, Affromumom korarima and Lippa Adonesis var. Koseret sebsebe were found to be very good sources of essential trace elements like Fe, Zn and Mn. The highest concentrat - ion of Mg was found in Ajowan whereas K and Fe were measured in Coriander seeds. The average daily dietary intake of some essential elements from the use of these spices were found to be below the recommended upper limit by WHO.

Key words: Spices; Herbs; essential elements; INAA

Elemental Characterization of Indigenous Food Cereal, Hordeum volgare, using Neutron Activation Analysis Technique and Gamma Ray Spectrometry

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Abstract

This study intended to assess the elemental characterization of plant cereal Hordeum volgare, that has served as staple food by all Ethiopian women during the period of post child delivery and lactating period for the first three months or more and also monitoring for some toxic elements, if any. The study identified essential and trace elements, in the sample, that support health and enhance nutritional value. Neutron activation analysis of indigenous white barely was done on sample collected directly from Shola which is one of largest indigenous cereals markets in Addis Ababa, Ethiopia. The experiment was carried out at the Czech Republic, using LVR15 research reactor at the CANAM infrastructure of NPICAS, Rez. The irradiated samples were analyzed using high purity Germanium detector and Gamma ray spectrometry and more than 40 elements were contained in the indigenous Ethiopian Cereal Hordeum volgare and most of the identified elements in considerable concentrations were essential elements for human health, in major, minor, and trace levels.

Key words: Hordeum volgare NAA(INAA), cereal sample, major, minor, and trace elements.