

International Conference on Physics Horizons and
Multidisciplinary Sciences (ICPHMS) 2025

Department of Physics COMSATS University Islamabad

9/01/2025

Editors:

Dr. Abdul Sattar (COMSATS University Islamabad)

Kashif Rehman (COMSATS University Islamabad)

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Abstracts

2D Materials: path toward new phenomena

Pawel J. Kowalczyk

University of Lodz

Recently, growing interest in 2D materials is observed initiated by exfoliation of graphene followed by investigations of silicane, germanene and stanene all located in 14th group of periodic table. Elements located in 15th group also crystalize in 2D form in layered A17 structure (black phosphorus structure, -form). The widely investigated -phosphorene is best known example, however, -arsenene, -antimonene, -bismuthene and -bismuth antimonidene can be synthesized. Interestingly, Sb and Bi can also form stable hexagonal form i.e. phase based on A7 structure (blue phosphorus). After successive synthesis of these materials we investigated their properties and over years we found number of interesting phenomena including unpinned Dirac states [1], nonsymorphic symmetries leading to formation of Dirac points [2], possible topologically protected edge states [3] and recently superlubricity and signatures of Levy flights in spontaneous diffusion of Bi on graphite [4]. The other group of 2D materials is based on transition metal dichalcogenide (TMDC) compounds. From this large group we will focus on TaS₂ and WTe₂ and their hybrids with graphene. These preliminary research show presence of variety of moire patterns indicating great platform for twistronics. We will also briefly discuss ageing and laser induced modification of MoTe₂, WTe₂ and BiTeCl. Finally, graphene can serve as electrode in many applications. To use it in photovoltaics its work function (WF) has to be substantially increased. We started series of experiments with 2D oxide MoO₃ growth [4, 5] which allowed us to tune graphene WF and create first working OLED in Poland. All these experiments are conducted using surface sensitive techniques including SPM and ARPES. Some of the experiments were conducted with LEEM/PEEM and STXM which are available only at synchrotron facilities. References [1] Q. Lu et al., Nat. Comm. 13 (2022) 4603 [2] P.J. Kowalczyk et al., ACS Nano 14 (2020) 1888 [3] S. Salehitaleghani et al., 2D Mat. 10 (2022) 15020 [4] M. Le Ster et al., arXiv 2406.16709, <https://doi.org/10.48550/arXiv.2406.16709> [5] D. Kowalczyk et al., 2D Mat. 8 (2021) 25005 [6] D. Kowalczyk et al., ACS Appl. Mat. Int. 14 (2022) 44506 Acknowledgments This work was possible thanks to National Science Centre, Poland under projects: 2020/37/B/ST5/03929 (OLED), 2019/35/B/ST5/03956 (Bi, Sb), 2018/31/B/ST3/02450 (TMDC)

The Future of Thin Film Coatings: A Scientific Review of Applications in Defense, Medicine and Electronics

Hakan Ates

Ghazi University Turkiye

Thin film coatings, with their nanometer-scale thickness and customizable properties, are central to modern materials science. These coatings play crucial roles, especially in defense, medical and electronics fields. This article / in the context of this keynote speech examines the current and potential future applications of thin film coatings in these two domains, discusses the manufacturing techniques used, and explores / attempts to pu forward the scientific and engineering perspectives for future advancements. Additionally, it covers the topic of flexible thin-film transistors and other advanced applications.

Tunning Electrical Conductivity of Graphene Composite Bi, CO, Co-doped LaFeO3 for Energy Storage Application

M. Fakhar-e-Alam

GCU Faisalabad

The development of effective energy storage systems is vital for solving the issues presented by the intermittency of renewable energy sources and the rising worldwide need for sustainable energy solutions. In this study, Lanthanum Ferrite (LaFeO₃), a perovskite oxide, is doped with Bismuth (Bi) and Cobalt (Co) using the co-precipitation approach, hoping to boost its electrochemical performance for energy storage applications. Lanthanum Ferrite is recognized for its chemical stability and modest electrical conductivity, although its performance may be considerably increased with selective doping. Cobalt is added to increase redox characteristics and electrical conductivity, while Bismuth promotes oxygen vacancy formation, allowing ionic transport. The co-precipitation process is adopted owing to its capacity to create homogeneously doped materials with controlled morphology and high purity, crucial for energy storage devices. The synthesized Bi and Co-doped LaFeO₃ materials are studied using structural, morphological, and electrochemical investigations to assess their applicability for supercapacitors and rechargeable batteries. This study addresses a large gap in the current literature by examining the combined effects of Bismuth and Cobalt doping in LaFeO₃, where little investigations have been undertaken. The discoveries are likely to give useful insights into the design of perovskite-based materials, leading to the development of high-performance energy storage devices that are crucial for the future of renewable energy technologies.

Influence of chloride ion on the morphology of electrodeposited Ni films

Ayesha Mubshrah

University of Bristol, UK

Electrodeposited nickel layers are extensively used for functional and decorative purposes e.g. the protective coating of spacecraft components[1]. The microstructure and morphology of thin electrodeposited metal films plays a vital role in determining their properties. We prepared a range of electrodeposited polycrystalline Ni films using potentiostatic deposition and investigated the effects of different parameters, such as the deposition rate, electrolyte composition. We characterized the surface morphology using ex-situ atomic force microscopy (AFM), We used the ex-situ AFM data to perform quantitative surface analysis, including slope and scaling analysis[2] and grain area calculation, as a function of deposition time and chloride addition. Film texture was determined by XRD analysis. For thin films the $\{111\}$ orientation was dominant, but for thick films, the dominant crystallographic orientation was $\{100\}$. We also performed electron backscatter diffraction (EBSD) analysis on the electrodeposited Ni thin films, using focused ion beam milling to remove the uneven top surface and obtain clear Kikuchi patterns. EBSD uses backscattered electrons to provide information on the crystallographic orientation of the thin films. Misorientation angles of the film's grain structure were also calculated, and twinning was observed in the EBSD data. We also performed HS-AFM and EBSD scans for the same area of an electrodeposited Ni thin to correlate the morphology and microstructural properties. Morphological studies at different growth stages using HS-AFM will provide insights into the growth rates at various points. Further 3D EBSD scans helps us to reveal the microstructural properties at different level of growth.

References: [1] P. Priyadarshi, P. K. Katiyar, and R. Maurya, Journal of Materials Science, 2022, 57, 19179-19211, 10.1007/s10853-022-07809-1 [2] L. Liu, and W. Schwarzacher, Electrochemistry communications, 2013, 29, 52-54, 10.1016/j.elecom.2013.01.017

Investigating Energy Transfer Mechanism in M Star Atmosphere through HighFrequency Alfvén Waves with Finite Temperature Effects Using MHD Modeling

Dr. Syeda Noureen

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Government Murray Graduate College, Sialkot Examining the energy transmission mechanisms in the chromosphere and corona of M stars is crucial to understanding the heating and dynamics of their atmospheric layers. This paper focuses on the role of high-frequency Alfvén waves in moving energy from the chromosphere to the corona of M stars using magnetohydrodynamic (MHD) models to account for finite temperature effects. By numerically solving the MHD equations, we examine the spatiotemporal energy transport enabled by these waves under different plasma

variables, such as density, temperature, and magnetic field intensity. The formation and maintenance of a stable corona surrounding M stars is examined by analyzing the changes in energy flux in space and time. The present findings offer critical insights into the energy balance in stellar settings and its dependence on plasma parameters, shedding light on the role of high-frequency Alfvén waves in atmospheric heating. Moreover, this work contributes to recognizing the basic processes driving M star atmospheres by highlighting the significance of temperature effects in wave propagation and energy dissipation

Exceptional ion conducting Amorphous solid solution of Yttrium-alumina Electrolyte for Low-Temperature Ceramic Fuel Cells

Hafsa Mansha

Southeast University Nanjing, China

The development of highly ion-conductive materials, particularly amorphous oxides at low temperatures, is critical for advancing low-temperature ceramic fuel cells (LT-CFCs). Despite their potential, the mechanisms behind the superior ionic conductivity of amorphous oxides remain a subject of significant scientific debate. A deeper understanding is essential to optimize their application and drive progress in CFC technology. In this study, we present an innovative amorphous electrolyte, Y-alumina, to explore ionic and proton conduction within the temperature range of 550°C–425°C. The 20 percent Y-alumina sample demonstrates exceptional performance, achieving high ionic conductivity of 0.25 S/cm and a remarkable power density of 1020 mW/cm² at 550°C. The disordered atomic structure of amorphous Y-alumina, combined with non-oriented grain boundaries (GBs), facilitates the generation of oxygen vacancies (Ov), reduces energy barriers, and enhances ionic mobility, enabling efficient ionic and proton conduction on its surface. A range of advanced characterization techniques, including X-ray diffraction (XRD), scanning and transmission electron microscopy (SEM and HR-TEM), X-ray photoelectron spectroscopy (XPS), and Thermogravimetric analysis (TGA), confirms the promising structural, morphological, and electrical properties of the amorphous Y-alumina. Furthermore, the study investigates ionic transport pathways, demonstrating how the disordered atomic configuration of amorphous oxides enhances both ion and proton transport. These findings establish Y-alumina as a highly promising amorphous oxide (AO) and a potential breakthrough electrolyte for LT-CFCs, paving the way for the innovative design and application of amorphous materials in next-generation ceramic fuel cells.

Hydrogen fuel cell optimization by machine learning

Hafsa Waheed, Prof. Rizwan Raza

COMSATS University Islamabad, Lahore Campus

Hydrogen has been hailed as a green fuel of the future that could end the world's dependence on fossil fuels and aid the transition of net zero emission. Hydrogen energy is sustainable since it can be generated from renewable and non-renewable energy sources such as water electrolysis, gasification of coal and other heavy hydrocarbons, direct and indirect thermochemical. Hydrogen fuel cell is a promising application in electricity generation through electrochemical process and water as a by product. It can be utilized in various sectors such as transportation, commercial, institutional, and residential. However, optimizing the performance of a fuel cell is a complex task, as it involves many interactive variables and non-linear dynamics. Therefore, machine learning is found to be a potent computational tool to study different characteristics and complex interactions and variables in a fuel cell. Machine learning algorithm can analyse large historical datasets from fuel cell operations and other parameters including material selection, chemical reaction modelling, polarization curves temperature, pressure, humidity, flow rates and other parameters, thus enabling more accurate predications of fuel cell operations under different operating conditions. This idea currently is now prevailing in most of the energy sector-based companies. In the short term, there is a great potential for hydrogen revolution, thus playing a big role in a decarbonised society in future.

Polyethylene glycol dictates the therapeutic response (anticancer and wound healing) of silver oxide nanomaterial

Husnain Ahmad

University of Punjab

This study focuses on WASP-2b, a hot Jupiter exoplanet, utilizing multi-wavelength photometry and light curve modeling to refine the planetary system's parameters and explore its atmospheric characteristics. Observations were conducted over two nights during the planet's transit using V, B, R, and I filters. The time-series data were calibrated and processed with AstroImageJ, and light curve modeling was performed using NASA's EXOFAST. Planetary parameters were derived from the best-fit data, with most results aligning well with published findings, except for specific discrepancies that shed new light on WASP-2b's transit properties. Notably, the results suggest potential wavelength-dependent variations in transit depth, offering hints of atmospheric features or stellar activity.

Synthesis of cobalt sulfide-nickel sulfide thin films via spray pyrolysis and their electrocatalytic applications

Jannat Farooq

^aFaculty of Engineering Sciences, Ghulam Ishaq Khan Institute of Engineering Sciences and Technology, Topi, Swabi, Khyber Pakhtunkhwa, Pakista

The development of highly efficient electrocatalysts from non-noble metal compounds through simple methods is crucial for effective water electrolysis and hydrogen energy production. However, choosing suitable materials with the right properties is highly challenging. Amorphous NiS-CoS thin films were grown on nickel foam in different mole ratios by using step, binder-free and cost-effective spray pyrolysis technique. The films growth were prepared by the reaction of aqueous solutions of nickel (II) acetate ($C_4H_6NiO_4$) and cobalt (II) acetate ($Co(CH_3CO_2)_2 \cdot 4 H_2O$) with thiourea on substrate heated to a temperature of $350 \pm 10^\circ C$. Surface morphology, structure and elemental composition of the thin films were investigated by scanning electron microscopy (SEM) and X-ray diffraction and Energy-dispersive X-ray spectroscopy (EDX). The prepared films were employed as promising electrocatalysts for the water splitting process. The catalytic activity and durability films were examined in 1 M KOH solution for HER. It has been observed that NiS-CoS thin films containing NiS content (75 percent showed the highest catalytic activity. The electrochemical analysis showed lowest overpotential at -20 mA cm^2 with lowest Tafel slope value for hydrogen evolution reaction (HER) making films compatible towards electrocatalysis of water in alkaline media than single components. It indicates that the HER performance of electrocatalyst can be enhanced by synergistic effect between NiS and CoS atoms. The as-prepared catalyst showed remarkable stability up to 5 h. Meanwhile, NiS-CoS thin films with 75 percent at Ni exhibits the highest activity with regard to the electrochemical surface area (ECSA).

Monte Carlo simulations of multiple-secondary cosmic ray detection by neutron detectors in Mawson Station, Antarctica

Mehak Kanwal ^{a,*}Alejandro Sáiz,^a Suttiwat Madlee,^b David Ruffolo,^a Warit Mitthumsiria

^a

Department of Physics, Faculty of Science, Mahidol University, Bangkok, Thailand
^b Department of Physics, Faculty of Science, Ramkhamhaeng University, Bangkok, Thailand
Galactic Cosmic Rays (GCR) are high energy particles or gamma rays from outside the Solar System. When they enter into our atmosphere, GCRs create secondary particle showers that can reach ground level. These showers can give us information about variations in the cosmic ray flux and spectrum, which in turn relate to solar activity. Neutron monitors (NMs) are basic instruments to measure such variations in the range of 1–100 GeV. To analyse timing data in a NM operating with updated electronics, it is important to know the relative time delays

and relative positions of multiple secondary particles produced by the same primary particle. So, in this work, we performed atmospheric Monte Carlo Simulations using Fluka version 4-4.0, and made a library of secondary particles produced in the atmosphere by each primary, storing their relative time and position information. Our future work will be to apply this model to the real data from neutron detectors at Mawson station (Australian Antarctic Territory) to compare with and validate our results. We gratefully acknowledge the logistical support provided by Australia's Antarctic Program for operating the Mawson neutron monitor. This research was also supported by a Postgraduate Scholarship from the Mahidol University Faculty of Graduate Studies, by Thailand's Office of the Permanent Secretary, Ministry of Higher Education, Science, Research and Innovation (OPS MHESI, Grant No. RGNS 65-181), by Thailand's National Science and Technology Development Agency (NSTDA) and National Research Council of Thailand (NRCT) under the High-Potential Research Team Grant Program (N42A650868), and from the NSRF via the Program Management Unit for Human Resources Institutional Development, Research and Innovation (B39G670013).

HYDROTHERMAL SYNTHESIS OF MXENES/VANADIUM PENTOXIDE NANOHYBRIDS FOR ALCO-SENSING APPLICATIONS

Muhammad Danyal Zarin¹ Dr. Abdul Hakim Shah²

Department of Physics, Khushal Khan Khattak University 27200-karak, Khyber
Pakhtunkhwa, Pakistan

The current research focuses on the synthesis of nanocomposites materials using MXenes (Ti_3AlC_2) and vanadium pentoxide (V_2O_5) through a hydrothermal method. The purpose of this synthesis is to explore efficient sensors for detecting volatile organic compounds (VOCs). MXenes are a class of two-dimensional materials known for their excellent electrical conductivity and large surface area. Vanadium pentoxide, on the other hand, is a compound that exhibits semiconducting properties and has potential applications in sensing. Our aim is to combine the unique properties of MXenes and vanadium pentoxide to develop nanocomposites materials with enhanced sensing capabilities for VOCs. VOCs are organic compounds that can easily evaporate and are commonly found in various industrial processes, household products, and environmental pollutants. Efficient sensing of VOCs is crucial for environmental monitoring, industrial safety, and health-related applications. The synthesized materials is characterized for structural and phases, morphological, elemental composition, functional groups and gas sensing properties through XRD, SEM, EDX, FTIR, UV-Vis spectroscopy and gas sensing system SGS-8, respectively.

A Co-FeCo₈S₈ Electrode for High Current Density Water Electrolysis Under Constant and Fluctuating Power Supply

Muhammad Jahangir Khan

Tsinghua Berkeley Shenzhen Institute, Tsinghua University

The increasing demand for sustainable energy solutions has accelerated research into advanced water electrolysis systems for hydrogen production, a critical component of the global energy transition. However, traditional electrode materials often face challenges in achieving high current density performance with long-term stability under fluctuating power conditions, such as those from renewable energy sources. On the one hand, conventional catalyst designs struggle to sustain industrial-scale current densities due to chemical and mechanical degradation. On the other hand, the integration of water electrolyzers with renewable energy systems necessitates materials that are both durable and efficient. Transition metal sulfides (TMSs) have emerged as promising materials for the oxygen evolution reaction (OER) due to their excellent electronic properties and abundant active sites. This project focuses on a monolithic Co-FeCo₈S₈ electrode synthesized via a solid-phase reaction, achieving high activity and stability at current densities above 2,000 mA cm⁻². Enhanced electron transfer, surface reconstruction during OER, and a robust catalyst-substrate bond ensure superior performance. The electrode's integration into a solar-powered anion exchange membrane water electrolyzer (AEMWE) addresses challenges of fluctuating renewable energy supplies, offering a scalable solution for sustainable hydrogen production.

First Principles Investigation of the Structural, Electronic, and Optical Properties of g-C₃N₄/HfSSe Heterostructure

NABEEL ANJUM, MUHAMMAD KASHIF, AAMIR SHAHZAD

Physics Department, Govt. College University Faisalabad (GCUF), Allama Iqbal Road, Faisalabad 38000, Pakistan

Heterostructures based on two-dimensional (2D) materials have gained remarkable attention because of their potential applications in various fields, such as electronics, optoelectronics, and catalysis. In the current study, we presented a comprehensive first-principles study on the structural, electronic and optical properties of heterostructures consisting of graphitic-carbon nitride (g-C₃N₄) and Janus HfSSe monolayer. Band structure analysis using HSE06 functional shows that g-C₃N₄/HfSSe heterostructure has a direct band gap of 0.31 eV and band edge analysis exhibited type-I band alignment suitable for optoelectronic applications. In the visible and ultraviolet spectrums, g-CN/HfSSe heterojunctions exhibit light absorption, which enhances solar energy absorption efficiency and broadens the range of optical responsiveness. Additionally, we studied the effect of strain on the band gap and optical properties. We observed vertical strain significantly changes the band gap and the optical absorption of the g-C₃N₄/HfSSe heterostructure. Our findings contributed to a fundamental understanding of 2D heterostructures based on Janus

materials and highlighted their promising prospects for future nanoelectronic and optoelectronic device applications

High Entropy Oxide material Enabling High Ionic Transport at Low Temperature Ceramic Fuel Cells

Muhammad Khalid, Rizwan Raza, Bin Zhu, MAK Yousaf Shah, Prof Jun Wang

Jiangsu Provincial Key Laboratory of Solar Energy Science and Technology/Energy Storage Joint Research Center, School of Energy and Environment, Southeast University, No.2 Si Pai Lou, Nanjing, 210096, China

High entropy oxides (HEOs) have garnered significant attention due to their promising applications across various fields, particularly in energy-related technologies. However, their potential in solid oxide fuel cells (SOFCs) remains largely underexplored. In this study, we present a novel approach to enhance ionic transport in SOFCs by introducing a local entropy gradient. A sol-gel method was employed to prepare a perovskite oxide HEO. In this article, we successfully synthesize five-element high-entropy oxides. The results showed that the HEO exhibited a significantly reduced polarization resistance (R_p) of 0.24 cm^2 at 520°C . When integrated into fuel cell devices, the HEO powders achieved a maximum power density of 580 mWcm^2 , accompanied by an open circuit voltage (OCV) of 1.07 V at 520°C . We propose that the local entropy gradient induced by the HEO enhances ion transport through the creation of a built-in electric field. This study provides valuable insights into the enhanced performance of HEO materials and offers new strategies for designing advanced materials with improved ionic transport properties for SOFC applications. Electrochemical impedance spectroscopy (EIS) and distribution of relaxation times (DRT) analyses further identified reduced resistance across the electrolyte interface, demonstrating the HEO's superior catalytic function. This work highlights the potential of HEO-based electrolyte to significantly improve LT-CFCs' performance by leveraging high configurational entropy for enhanced material properties. These insights highlight the critical role of HEO in optimizing the electrocatalytic performance of FCs, underscoring its significant importance in advancing FC technology

Polyethylene glycol dictates the therapeutic response (anticancer and wound healing) of silver oxide nanomaterial

Muhammad Khawar
GC University Faisalabad

In this study, polymer (polyethylene glycol [PEG] and Chitosan)-coated silver oxide nanoparticles (NPs) have been prepared by hydrothermal method. The polymer encapsulated NPs are characterized by materials-related characterization techniques such as X-Ray diffraction (XRD), scanning electron microscope (SEM), Ultraviolet-visible (UV-Vis), photoluminescence (PL), and Fourier-transform infrared (FTIR) spectroscopy. The crystallite size of silver oxide NPs is 43.39 nm and reduces to 34.56 nm and 30.43 nm for PEG and Chitosan functionalized NPs, respectively. SEM micrographs show the spherical morphology of the synthesized nanomaterials with the grain size of pristine, PEG, and Chitosan functionalized silver oxide NPs as 60.9 ± 14.1 , 70.9 ± 10.3 , and 57.2 ± 7.8 nm, respectively. The band gap of silver oxide NPs increases upon polymer functionalization. PEGylation of silver oxide NPs has enhanced its anticancer potential significantly against liver cancer cell line (HuH-7), shows least cell viability, and IC₅₀ value is as low as 0.106 g/mL and in the case of Chitosan coating 4.505 g/mL. The antibacterial properties and biofilm inhibition are investigated against bacterial extracts of *Escherichia coli* and *Staphylococcus aureus*. The polymer-coated silver oxide NPs have shown enhanced antibacterial potential against both *S. aureus* and *E. coli*. CAM assay is used to evaluate the wound-healing ability of nanomaterials. Alginate gels incorporated with NPs have promoted wound healing. Our results revealed that the surface modification by PEG and Chitosan improved the therapeutic potential of silver oxide NPs.

Characterization and Synthesis of Carbon based structures on Copper Substrates by Radiofrequency Inductively Coupled Plasma

Muhammad Zaman and Hafeez Anwar
ANDL Lab., Department of Physics, University of Agriculture Faisalabad

Devices for storing energy are new developments developed to collect and conserve energy for use in the future. These consist of capacitors, batteries, supercapacitors and other devices which store energies i-e thermal, chemical or energy from electricity. Such instruments are vital for regulating the demand and supply of energy particularly in energy from renewable sources. Electrodes of supercapacitor devices serve as vital for storing energy because they offer a large area needed for charge collection. The aim of this research was to deposit carbon on copper substrate by inductively coupled plasma for material of electrode. Copper substrates were sonified by mixing isopropanol with deionized water. Argon gas was used as carrier gas and precursor acetylene used as carbon source. Prepared samples were characterized by using various techniques like XRD, SEM, Raman spectroscopy and Cyclic Voltammetry. XRD was used for studying the structure of crystals by examining

the patterns of diffraction of an X-ray that interact with copper substrate. SEM was employed to examine the surface of copper substrate. Raman spectroscopy was used to study details about chemical structure and vibrations of molecules of copper substrate. Cyclic voltammetry was used for fluctuating voltage and monitoring the electrical current in order to examine the redox features of copper substrate. Carbon was deposited perfectly on copper substrate and show promising application in supercapacitor as material of electrode.

Nickel oxide-Cobalt oxide Thin Film Deposited on Ni Foam by Spray Pyrolysis for Enhanced Electrochemical Water Splitting

Mushabbah Ashfaq a, Farhat Yasmeen a, Iqra Muneer a, Dilawar Ali b, Jannat Farooq a, Samina Farid a

a Department of Chemistry, University of Engineering and Technology, Lahore, 54890, Pakistan b Department of Physics, GC University, Lahore, Lahore-54000, Pakistan

Developing cost-effective, efficient, and durable oxygen evolution reaction (OER) electrocatalysts composed of earth-abundant elements through simple synthesis methods is critical for green hydrogen production via water electrolysis. In this study, thin films of nickel oxide, cobalt oxide and nickel oxide-cobalt oxide nanocomposites thin films in ratios of 1:1, 1:3, and 3:1 were fabricated on a Ni foam substrate using a straightforward spray pyrolysis technique at $350 \pm 5^\circ\text{C}$. These thin films, exhibiting comparable surface morphologies, were characterized via SEM-EDX, FTIR, and XRD to determine their structural features and assess their OER activity. Among the compositions tested, the Nickel oxide-cobalt oxide thin film with a 3:1 ratio exhibited the lowest overpotential to reach the standard current density of 10 mA cm^{-2} and the lowest Tafel slope which is comparable to the performance of commercial RuO catalysts. The enhanced OER performance of the Nickel oxide-cobalt oxide nanocomposite electrocatalysts system can be ascribed to the synergistic interactions and electronic modifications between Ni and Co atoms, effectively lowering the energy barrier for OER. The chronoamperometry results demonstrated excellent stability, maintaining performance for up to 5 hours. Additionally, electrochemical impedance spectroscopy (EIS) revealed a low resistance value indicating efficient charge transfer. Hence, the nickel oxide-cobalt oxide thin films prepared by this facile synthesis route hold promise as efficient and low-cost electrocatalysts for industrial-scale green hydrogen generation via water electrolysis.

First Principles Investigation of the Structural, Electronic, and Optical Properties of g-C₃N₄/HfSSe Heterostructure

Dr. Muhammad Sharif

ANDL Lab., Department of Physics, University of Agriculture Faisalabad

Devices for storing energy are new developments developed to collect and conserve energy for use in the future. These consist of capacitors, batteries, supercapacitors and other devices which store energies i-e thermal, chemical or energy from electricity. Such instruments are vital for regulating the demand and supply of energy particularly in energy from renewable sources. Electrodes of supercapacitor devices serve as vital for storing energy because they offer a large area needed for charge collection. The aim of this research was to deposit carbon on copper substrate by inductively coupled plasma for material of electrode. Copper substrates were sonified by mixing isopropanol with deionized water. Argon gas was used as carrier gas and precursor acetylene used as carbon source. Prepared samples were characterized by using various techniques like XRD, SEM, Raman spectroscopy and Cyclic Voltammetry. XRD was used for studying the structure of crystals by examining the patterns of diffraction of an X-ray that interact with copper substrate. SEM was employed to examine the surface of copper substrate. Raman spectroscopy was used used to study details about chemical structure and vibrations of molecules of copper substrate. Cyclic voltammetry was used used for fluctuating voltage and monitoring the electrical current in order to examine the redox features of copper substrate. Carbon was deposited perfectly on copper substrate and show promising application in supercapacitor as material of electrode.

Advancing X-ray Polarimetry: Insights from IXPE and Future Prospects

Saba Imtiaz

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talian National Institute for Astrophysics (INAF) , Roma,Italy Imaging X ray polarimetry explorer (IXPE) has opened a new window in astrophysics by providing precise X-ray polarimetry for a diverse sample of celestial sources. Both Radio Quiet and Radio Loud AGNs, as well as galactic black hole binaries and neutron stars, have been probed. For the first time, polarization maps in X-rays of pulsar wind nebulae and supernova remnants have been made available. Additionally, faint extended sources, such as molecular clouds and filaments around the Galactic Center and near lobes from microquasars, have been successfully investigated. Although theoretical models were sometimes confirmed, IXPE has reported, for many observations, unexpected results that warrant further and deeper investigation by theorists on one hand, and, on the other a new mission with improved polarimetric capabilities. Now we are working on some possible new directions beyond IXPE.

Boosting Optoelectronic Performance of Green LEDs with DualStage Interlayer Integration

Shazma Ali a*, Muhammad Usmana, Anum Alia, Zoya Noora

aFaculty of Engineering Sciences, Ghulam Ishaq Khan Institute of Engineering Sciences and Technology, Topi, 23460, Khyber Pakhtunkhwa, Pakistan.

Micro-light-emitting diodes (LEDs) have great potential to revolutionize fields such as display technology, lighting, and biomedical devices due to their excellent performance, flexibility, high brightness, and energy efficiency. Despite these advantages, the advancement of LEDs is hindered by several challenges, with surface defects posing a major obstacle to achieving high internal quantum efficiency (IQE). These defects facilitate charge carrier recombination at nonradiative sites, significantly reducing IQE and overall device performance. This issue becomes more pronounced in LEDs due to their diminutive size and elevated surface-to-volume ratio, making it a critical issue to address. Researchers have explored various approaches to numerically enhance the performance of Gallium Nitride (GaN)-based LEDs. This research focuses on numerically enhancing the optoelectronic performance of GaN-based green LEDs by incorporating a dual-stage interlayer (GaN/AlGaN) within the p-region. The introduction of this interlayer alters the bandgap energy and electric field, which facilitates the acceleration of holes toward the active region while minimizing their trapping at surface defects. Consequently, the radiative recombination rate significantly improves. The results demonstrate an increase in peak internal quantum efficiency (IQE) by up to 60 percent, along with an output power enhancement to 47 W/m. Additionally, the emission intensity surpasses that of conventional designs.

Study Of Structural, Optical and Electrical Properties Of ZN/MWCNTs/rGOMOS2/ Nanocomposite For Their Supercapacitor Applications.

Shazma Shahid

Department of Physics Cosmsats university Islamabad, Lahore Campus, Pakistan

MoS₂ is a material which belongs to the transition metal dichalcogenides (TMDC) family having the chemical formula MX₂. It is the most promising material after graphene. MoS₂ and rGO as well as MWCNTs is the most researched material among numerous materials due to its excellent optical, mechanical and electrical properties. Their compounds with different metals show outstanding performance in electrochemical and supercapacitive applications. Zn/MWCMTs/rGO/MoS₂ nanocomposites have been synthesized by Sol-Gel technique. To assess several characteristics of synthesized materials different characterization techniques such as X-ray Diffraction (XRD), Fourier Transformation Infrared Spectroscopy (FTIR), UV-Visible (UV-Vis.) spectroscopy and Scanning Electron Microscopy (SEM) were applied. The XRD patterns shows the Hexagonal structure confirming the successful formation of the material. The Scherrer formula, Williamson-Hall, and Scherrer

plot methods were used to calculate crystallite size and lattice strain. The average crystallite size was measured using these methods. Furthermore, the optical properties such as absorption and bandgap of the fabricated nano-material and composites were determined by UV-Vis. Spectroscopy. The observed band gap for MWCNTs/GO/MoS2 and Zn doped MWCNTs/rGO/MoS2 nano-composite different absorption peaks were observed having specific bandgap values. The successful synthesis of nanocomposites was also confirmed by FTIR analysis. Different stretching vibration belongs to MWCNTs, GO and Zn were observed. SEM indicates the sheets like morphology of the synthesized composite showing a net of MWCNTs and Zn nano-spheres. CV and EIS measurements indicates the good electrochemical performance of the synthesized material. The electrode's supercapacitive measurements reveal a high specific capacitance of 970 F/g at 10mV/s. EIS measurements were taken from "Nquist" plot indicating a decrease in resistances of modified electrodes of the samples. The impedance in MWCNTs/GO/MoS2 nanocomposite reduced to 1/4th than the undoped composites.

Polymer Capped Iron Oxide Nanoparticles for Biomedical Applications

Tariq Munir¹, Arslan Mahmood¹, Azhar Rasul²

¹Department of Physics, Government College University Faisalabad (GCUF), Allama Iqbal Road, Faisalabad, 38000, Pakistan, ² Department of Zoology, Government College University Faisalabad (GCUF), Allama Iqbal Road, Faisalabad, 38000, Pakistan

Polymer capped transition metal oxide nanoparticles (TMO-NPs) are becoming a major thrust of modern research due to potential application in antibacterial and anticancer activity. The polymer capping agents such as Citric acid, Malic acid are used to enhance the sensitivity and played the vital role to control the size, morphology and monodispersity of TMO-NPs. The present study will be related to synthesis of pure and capped Fe₃O₄ NPs by using chemical method. The prepared Iron oxide-NPs will be characterized by using various characterization techniques such as XRD, SEM, FTIR, VSM and in vitro and in vivo bioassay. The XRD will be preferred to identify the crystal structure and also used to calculate the crystallite size of pure and capped Fe₃O₄ -NPs. The SEM analysis will be used to investigate the surface morphology. The FTIR will be measured the different functional groups attached on the surface of NPs. Moreover, the VSM analysis will be performed to measure the magnetization power of pure and capped Fe₃O₄-NPs. At the end material related study will be provided the information about the Fe₃O₄-NPs is suitable for antibacterial and anticancer activity.

Unveiling exceptional Conduction mechanism and High proton conductivity in Amorphous Electrolyte for Advanced Ceramic Fuel Cells

Touseef Ahmad

Southeast University Nanjing, China

The requirement of high ion conductive material working at low temperature is highly demanding in fuel cell. This study explains a novel groundbreaking advancement in ceramic fuel cells by exploring the potential of amorphous Sm_{0.3}Al_{0.7}-oxide and the proton conduction mechanism of amorphous oxides. Opposite to conventional crystalline electrolytes, amorphous electrolytes showed superior ion conduction, to study detailed mechanism of ion conduction amorphous Sm_{0.3}Al_{0.7}-oxide was selected which exhibited an exceptional proton conductivity of 0.17 S/cm and a power density of 1100 mW/cm² at 550 °C, significantly surpassing traditional electrolyte materials. Using advance characterizations techniques, a new approach has been proposed to provide the reasons for high conductivity of amorphous materials which entailed a complete mechanism that describe how disordered structure and disoriented grain boundaries facilitate efficient proton conduction by reducing energy barriers and enhancing ionic mobility. Also it has been described how the high enthalpy and the high energy state of amorphous materials is suitable for enhancing proton conduction. This study aims to clarify why amorphous materials are promising candidates for future fuel cell applications, facilitating significant advancements in SOFC and PCFC technologies and paving the way for more efficient and sustainable energy solutions.

An Extensive Study of Structural, Electronic, Mechanical and Thermodynamic Properties of KCuH₃ for Hydrogen Storage Applications: First-Principles Approach

Zia-Ur-Rehman, Muhammad Jabran, Muhammad Numair

Department of Mathematics, Namal University, 30km Talagang Road, 42250, Mianwali, Pakistan.

The increasing global energy demands necessitate the exploration of sustainable and efficient hydrogen storage solutions. This study investigates the structural, electronic, mechanical, and thermodynamic properties of potassium-based hydride (KCuH₃) using density functional theory (DFT). The results reveal that KCuH₃ compounds exhibit cubic crystal structures and belong to the Pm-3m space group, demonstrating a bulk modulus of 55.65 GPa, indicating superior mechanical stability. The gravimetric hydrogen storage capacity is calculated to be 2.861 percent for KCuH₃, confirming its potential as a viable hydrogen storage material. Additionally, the electronic band structure analysis indicates metallic behavior, which is favorable for hydrogen absorption and release. The desorption temperature, derived from the formation enthalpy and entropy change, is estimated to be 11,298 K for KCuH₃. This research provides a comprehensive understanding of the properties

of KCuH_3 , highlighting its potential for practical applications in hydrogen storage technologies

Exceptional ion conducting Amorphous solid solution of Yttrium-alumina Electrolyte for Low-Temperature Ceramic Fuel Cells

Hafsa Mansha

Southeast University Nanjing, China

The development of highly ion-conductive materials, particularly amorphous oxides at low temperatures, is critical for advancing low-temperature ceramic fuel cells (LT-CFCs). Despite their potential, the mechanisms behind the superior ionic conductivity of amorphous oxides remain a subject of significant scientific debate. A deeper understanding is essential to optimize their application and drive progress in CFC technology. In this study, we present an innovative amorphous electrolyte, Y-alumina, to explore ionic and proton conduction within the temperature range of 550°C – 425°C . The 20 percent Y-alumina sample demonstrates exceptional performance, achieving high ionic conductivity of 0.25 S/cm and a remarkable power density of 1020 mW/cm^2 at 550°C . The disordered atomic structure of amorphous Y-alumina, combined with non-oriented grain boundaries (GBs), facilitates the generation of oxygen vacancies (Ov), reduces energy barriers, and enhances ionic mobility, enabling efficient ionic and proton conduction on its surface. A range of advanced characterization techniques, including X-ray diffraction (XRD), scanning and transmission electron microscopy (SEM and HR-TEM), X-ray photoelectron spectroscopy (XPS), and Thermogravimetric analysis (TGA), confirms the promising structural, morphological, and electrical properties of the amorphous Y-alumina. Furthermore, the study investigates ionic transport pathways, demonstrating how the disordered atomic configuration of amorphous oxides enhances both ion and proton transport. These findings establish Y-alumina as a highly promising amorphous oxide (AO) and a potential breakthrough electrolyte for LT-CFCs, paving the way for the innovative design and application of amorphous materials in next-generation ceramic fuel cells.

Two-Stage Machine Learning Approach for Perovskite Bandgap Prediction: Comparing DFT-Calculated and Experimental Features

Zia-Ur-Rehman^{1*}, Anam Fatima²

¹Department of Mathematics, Namal University, 30km Talagang Road, 42250, Mianwali, Pakistan. ² Department of Computer Science, Namal University, 30km Talagang Road, 42250, Mianwali, Pakistan.

Perovskite materials have become an emerging class due to their wide range of applications in various fields including solar cells, lasers, memory devices, and photovoltaics. Accurate prediction of their bandgap can reduce the time for finding the best material for a desired application. Although traditional methods like Density Functional Theory (DFT) can accurately predict bandgap, they are computationally expensive and highly time-consuming. This study proposes a two-stage machine learning technique to accurately and quickly predict the bandgap of perovskites. The properties of 3,610 materials were obtained from the Materials Project database. In our two-stage machine learning technique, the first stage comprises a classification model that categorizes materials into direct or indirect bandgap types. The second stage involves a regression model to predict the electronic bandgap value. The dataset is divided into two experimental classes: one containing complex DFT-calculated features and the other containing only experimentally determined features. After benchmarking several state-of-the-art machine learning algorithms, Random Forest emerged as the optimal choice for both classification and regression tasks. Using Random Forest, the classification model achieved an accuracy of 84.9 percent on the first dataset (with DFT-calculated features) and 84.7 percent on the second dataset, while regression yielded a mean absolute error of 0.32 eV for the first dataset and 0.41 eV for the second one. These small variations in results demonstrate that bandgap can be accurately predicted using experimental features alone.

A Simulation Study of the Princess Sirindhorn Neutron Monitor's Response to Solar Neutrons

Areej Kazmi, Warit Mitthumsiri, Alejandro S´aiz, David Ruffulo

Department of Physics, Faculty of Science, Mahidol University, Bangkok, Thailand

Solar Energetic Particles are lower-energy cosmic rays that interact with the Earth's atmosphere to produce secondary particles, including neutrons. In this research, we investigate the response of the Princess Sirindhorn Neutron Monitor (PSNM) to solar neutrons, which originate from solar activities such as solar flares and coronal mass ejections. The PSNM, located at the equator with a high cut-off rigidity of 16.7 GV, is particularly suited for this study as it effectively detects solar neutrons penetrating the atmosphere. The research involves simulating large numbers of solar neutrons at different zenith angles and energies, followed by a comparison with real data from the PSNM. The methodology includes Monte Carlo simulations to model the interactions of solar neutrons with the atmosphere and the PSNM,

providing insights into detection mechanisms and the characteristics of these high-energy particles. This research is expected to contribute significantly to the fields of cosmic ray studies and solar physics.

Asima Sarwar

Gulam Ishaq Khan Institute of Engineering Science and Technology Topi Swabi

Deep ultraviolet (DUV) Aluminum Gallium Nitride (AlGaN)-based laser diodes (LDs) are traditionally designed using simulation software, which is often resource-intensive and time-consuming, thereby slowing down the design process. This study introduces a machine learning (ML)-based framework to streamline the design of AlGaN-based DUV LD structures. Using a dataset generated with SiLENSe™, incorporating variations in the thickness and composition of the waveguide, cladding, and electron blocking layer (EBL), five ML models were evaluated. Among these, the Extreme Gradient Boosting (XGB) model demonstrated the highest predictive accuracy, achieving R² scores of 85 percent for output power, 92 percent for threshold current, and 82 percent for optical confinement factor. Feature importance analysis, performed with SHapley Additive exPlanations (SHAP), identified the key structural parameters influencing LD performance, enabling explainable artificial intelligence (XAI). This ML-driven design methodology not only accelerates the development cycle but also facilitates the optimization of LD structures by guiding critical parameter selection during the manufacturing process.

Characterization and Synthesis of Carbon based structures on Copper Substrates by Radiofrequency Inductively Coupled Plasma

Dr. Muhammad Sharif

ANDL Lab., Department of Physics, University of Agriculture Faisalabad

Devices for storing energy are new developments developed to collect and conserve energy for use in the future. These consist of capacitors, batteries, supercapacitors and other devices which store energies i.e thermal, chemical or energy from electricity. Such instruments are vital for regulating the demand and supply of energy particularly in energy from renewable sources. Electrodes of supercapacitor devices serve as vital for storing energy because they offer a large area needed for charge collection. The aim of this research was to deposit carbon on copper substrate by inductively coupled plasma for material of electrode. Copper substrates were sonified by mixing isopropanol with deionized water. Argon gas was used as carrier gas and precursor acetylene used as carbon source. Prepared samples were characterized by using various techniques like XRD, SEM, Raman spectroscopy and Cyclic Voltammetry. XRD was used for studying the structure of crystals by examining the patterns of diffraction of an X-ray that interact with copper substrate. SEM

was employed to examine the surface of copper substrate. Raman spectroscopy was used used to study details about chemical structure and vibrations of molecules of copper substrate. Cyclic voltammetry was used used for fluctuating voltage and monitoring the electrical current in order to examine the redox features of copper substrate. Carbon was deposited perfectly on copper substrate and show promising application in supercapacitor as material of electrode.

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