

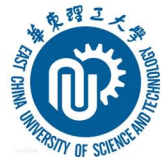


2nd International Symposium on Advanced Energy Materials:

ISAEM 2019

Production to Storage

10 December 2019





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Session 1:

Chair: Prof. Anila Asif

*Interdisciplinary Research Centre in
Biomedical Materials,
COMSATS University Islamabad, Lahore
Campus, Pakistan*

Co-Chair: Dr. Muzaffar Hussain

*Chair Department of Physics
Air University Islamabad, Pakistan*



Keynote Lecture

Prof. Jinlong Zhang

*School of Chemistry and Molecular
Engineering, East China University of Science
and Technology, Shanghai, China*



Keynote Lecture: Design and Preparation of Novel Photocatalytic Materials for Hydrogen Production

Prof. Jinlong Zhang

East China University of Science and Technology, Shanghai, China

Abstract

Solar energy driven photocatalytic water splitting into hydrogen over semiconductor photocatalysts has been considered as a clean and efficient technology to address the excessive consumption of fossil fuels. The potential success of the solar-to-hydrogen heavily depends on the development of efficient semiconductor photocatalysts which can achieve solar light harvesting, efficient separation of photogenerated electrons and holes and generate active electrons on the appropriate energy level for satisfying the redox process towards hydrogen evolution. Unfortunately, a single-component semiconductor is very difficult to meet all the above-mentioned requirements, because photogenerated electrons in the conductive band (CB) is inclined to be back to the valence band (VB), which seriously lower down the utilization efficiency of solar energy. To solve this dilemma, bio-inspired “artificial photosynthetic system”, a so-called direct Z-scheme photocatalytic process, has been developed through rational introduction of two different semiconductors without a reversible donor-acceptor pair. Here, we develop a new strategy for design and synthesis of Co₉S₈ hollow cubes decorated by CdS QDs hybrid Z-scheme system. The result shows that an efficient Z-scheme build block and the multiple reflections of solar light within the cavity of hollow cubes are responsible for the substantially enhanced HER activity and stability. Cd_xZn_{1-x}Se/CoP composites have been well studied as an effervescent photocatalyst for the H₂ evolution. The molar ratio of Cd/Zn, loading amount of CoP and concentration of sacrificial agent have been investigated. Under the optimal conditions, a high quantum yield of 11.8% at ~520 nm can be obtained. The absolute value of H₂ production quantity of 50 mg Cd_{0.25}Zn_{0.75}Se/CoP under the visible light (>420 nm) irradiation can be up to 1.2 mmol h⁻¹.



Invited Lecture: Fused ring Small Molecule Acceptors for High-performance Fullerene-free Organic Solar Cells

Raja Shahid Ashraf (MRSC)

Associate Professor, Department of Chemistry, Government College University, Lahore

Abstract

Solution-processed organic solar cells offer promising renewable energy conversion, due to low cost, low weight, and flexibility. Development of new materials and optimization of donor and acceptor interface of organic solar cells has driven efficiencies beyond 10% for single junction solar cells with bulk heterojunction architecture. Due to these arising issues of using fullerene derivatives, as acceptors such as; difficult synthesis, limited tunability of energy levels, high cost for purification, morphological instability and weak light absorption in the visible region. Fused ring non-fullerene small molecule acceptors have become more attractive recently due to their benefits of being easier to synthesize than fullerene-based acceptors and ability to gain excellent purity compared to polymers, chemical modifications allow for easy tuning of optical and electronic properties, good absorbance, good morphology and suitable for flexible devices. Recently, we have reported a series of the non-fullerene acceptor (IDTBR) containing IDT as a central core with efficiencies reaching 11%. Herein, we like to report a systematic modification of IDTBR acceptor structure. We have modified alkyl chains on the electron donating part indacenodithiophene (IDT) and replacement of acceptor end groups. Substitution of acceptor end groups resulted in the shift of energy levels and a shift in the absorption spectrum. We will discuss in detail the impact of a change in alkyl chain length and outer peripheral acceptors end group of these new molecules on optoelectronic properties. These new modified structures of IDTBR acceptors have shown promising performance in single junction solar cells with different donor polymers, resulting efficiencies were above 12%. OPV device performance, photophysics and morphological studies of these blends will be presented.

Oral Lecture: In-depth Study on How Energy Storage Technology Can be Used to Build Sustainable Energy Systems

Ahsan Ejaz

*Assistant Professor, Mirpur University of Science and Technology,
Mirpur city, Azad Kashmir, Pakistan*

Abstract

The aim of this work is to evaluate the electrochemical corrosion managements of Alloy 800 in the primary water reactor solution (PWR) with and without hydrogen, in the temperature range of 25-75 °C. Corrosion behavior of Alloy 800 was determined by using Open circuit potential measurements, anodic polarization, potentio static polarization, electrochemical impedance spectroscopy, Mott-Schokty plots, X-ray photoelectron spectroscopy and Scanning electron microscopy. OCP for the hydrogen-charged specimen was quite low than non-charged, anodic polarization for hydrogen-charged was higher than the non-charged especially in active and passive regions, for transpassive region both hydrogen-charged and non-charged exhibited almost same current density. Impedance for the hydrogen-charged specimen was decreases greatly, it showed a small second semi-circle, M-S plots indicates passive film formed on Alloy 800 was n-type semiconductor. XPS indicates Ni/Cr content decreases in the passive films that can be due to charged hydrogen have strong reaction with the vacancies present in the passive films. An equivalent circuit was used to fit and explain all the collected data for different conditions.



Oral Lecture: Electron Directed Migration Cooperated with Thermodynamic Regulation Over Bimetallic NiFeP/g-C₃N₄ for Enhanced Photocatalytic Hydrogen Evolution

Qiaohong Zhu

*East China University of Science and Technology, Shanghai, P.R
China*

Abstract

Bimetallic phosphides have attracted considerable attention in photocatalytic hydrogen evolution reaction (HER), owing to its thermodynamic feasibility. Most reports attributed the HER activity to the reduction of free energy of protonation (ΔGH^*), however, few revealed the whereabouts of the photo-induced electrons, which makes the mechanism of HER not very clear. Herein, nickel-iron bimetallic phosphide (NiFeP) is designed onto graphitic carbon nitride (NiFeP/g-C₃N₄) for the photocatalytic HER, which exhibits a high hydrogen production of 3.549 mmol g⁻¹ h⁻¹. It is found that the co-catalyst of NiFeP can not only reduce the ΔGH^* , but also make the photogenerated electrons transfer directionally, which play a synergistic role in enhancing the activity of HER. The reduction of ΔGH_2O and ΔGH^* over NiFeP in HER can be well demonstrated by the density functional theory (DFT) calculations. Furthermore, the localized distribution of electrons on the surface of NiFeP is verified by measuring the lifetime of photo-generated carriers combined with the REDOX experiment. The shortened lifetime τ , decreased τ^1 and τ^2 of NiFeP/g-C₃N₄ indicate that the photoexcited electrons of g-C₃N₄ are directly transferred to the co-catalyst surface, contributing to the worse delocalization capacity of electrons on the cocatalyst and its easier reactions with protons trapped on the co-catalyst surface. Besides, the density of state intensity (DOS) also confirms the photogenerated electron migration pathway at the metal-semiconductor (NiFeP/g-C₃N₄) interface. Our research clarifies the mechanism of bimetallic phosphides co-catalytic HER system, which will provide theoretical guidance for the design and preparation of multi-metallic center photocatalytic system with a higher HER activity in the future.



Oral Lecture: Using Microbial Fuel Cell as A Source for Sustainable Energy Production

Naeem Ullah

*Chairman, Department of Chemistry, University of Turbat,
Balochistan, Pakistan*

Abstract

This research used an open chamber mediator-less microbial fuel cell to convert the chemical energy into electrical energy by the fermentation of domestic wastewater through the use of yogurt. The wastewater sample was subjected to aerobic fermentation in a single and double chamber BFC for 7 days by using yogurt. Parallel and series combinations were also developed by using copper and zinc electrodes in single and double chamber BFC. The parallel and series combinations were based on four units of the single and double chamber BFC separated. The physical parameters such as pH, conductance, current density, voltage, power output and resistance were monitored for a week to observe changes due to metabolic activities of microorganisms. It was observed that the current density of the single unit was multiplied with the total number of units connected in a parallel combination. On the other hand, in the series combination the voltage of the one unit is multiplied by the voltage of the total number of the added units. The high current density (39.20 mA) was found in the parallel combination of single chamber open system BFC using eight electrodes each of zinc and copper. On the other hand, the high voltage (4.10 V) was found for the series combination of double chamber open system BFC using continuous-circuit bridge and two electrodes each of zinc and copper. These results showed that the fermentation of domestic wastewater with yogurt result in a valuable increased in electrical energy.

Oral Lecture: Synthesis and Characterization of Anode Materials for Low Temperature SOFCs

Khalil Ahmad^{a,b}, Ghazanfar Abbas^{a*}, M. Ashfaq Ahmad^a

^a *Department of Physics, COMSATS University Islamabad, Lahore
Campus-54000, Pakistan*

^b *Department of Physics, Virtual University of Pakistan*

Abstract

Fossil fuel-based energy assets are being used rapidly and the high utilization of these sources motivated the researchers and scientists and to look forward alternative energy conversion devices. Fuel cell is an electrochemical energy conversion device without the involvement of combustion process. Among fuel cell family, Solid oxide fuel cell which got considerable attention due to higher efficiency, environment friendly and fuel flexibility. Graphene incorporated composite anode materials have been prepared in the present work. Composite electrodes of $\text{Al}_{0.1}\text{Ni}_{0.2}\text{Zn}_{0.7}$ have been synthesized by solid state reaction method as anode material and different amount as 1, 1.3, and 1.5 wt.% of graphene is then incorporated in prepared composite material. XRD and SEM were employed to study the crystal structure and surface morphology. The crystallite sizes evaluated by XRD peaks are found in the range of 42-56 nm and results were found to nearly agree with SEM analysis. Electrical conductivity has been measured at the function of temperature from 300-650 °C by Four-Probe DC method and maximum value is found to be 0.53 Scm^{-1} at 370 °C with 1.3% of graphene incorporation. The peak power density was obtained 375 mWcm^{-2} at 600 °C with 1.3% graphene incorporation.



Session 2:

Chair: Prof. Jinlong Zhang

*School of Chemistry and Molecular
Engineering, East China University of Science
and Technology, Shanghai, China*

Co-Chair: Dr. Naeem Ullah

*Chair Department of Physics
University of Turbat, Balochistan, Pakistan*



Keynote Lecture

Prof. Lingzhi Wang

*School of Chemistry and Molecular
Engineering, East China University of Science
and Technology, Shanghai, China*

Keynote Lecture: Ga-doped and Pt-loaded Porous TiO₂-SiO₂ for Photocatalytic Nonoxidative Coupling of Methane

Lingzhi Wang

Key Lab for Advanced Materials and Institute of Fine Chemicals, East China University of Science and Technology; 130 Meilong Road, Shanghai, P. R. China

Abstract

Methane is a promising energy source with huge reserves and is considered as one of the alternatives to non-renewable petroleum resources, since it can be converted to valuable hydrocarbon feedstocks and hydrogen through appropriate reactions. Nonoxidative coupling of methane (NOCM) has proven to be a promising approach to methane conversion for C₂ products and hydrogen. However, a high activation temperature is required to trigger this reaction owing to the tremendous thermodynamic barrier, which often causes coke deactivation of the catalyst and low selectivity. Therefore, there is an urgent demand to develop new strategies for NOCM under mild conditions.

Herein, a Ga-doped TiO₂-SiO₂ microarray with a hierarchical macro-mesoporous structure (HGTS) is developed for NOCM. Pt nanoclusters, as a commonly used cocatalyst for the photocatalytic hydrogen evolution reaction, are further deposited (Pt/HGTS) to explore their effect on NOCM. A high CH₄ conversion rate of 3.48 μmolg⁻¹h⁻¹ for the selective production of C₂H₆ is achieved at room temperature. Moreover, a steady H₂ yield of 36 μmolg⁻¹ within 32 h is attained and is accompanied by a high CH₄ conversion percentage of 28% without loss of structural stability. The influence of Ga on the chemical state of a surface oxygen vacancy (Vo) and deposited Pt is investigated through a combination of experimental analysis and first-principles density functional theory calculations. Ga substitutes for the five-coordinated Ti next to Vo, which tends to stabilize the single-electron trapped Vo and reduce the electrons transfer from Vo to the adsorbed Pt, resulting in the formation of a higher amount of cationic Pt. The cationic Pt and electron-enriched metallic Pt form a cationic-anionic active pair, which is more efficient for the dissociation of C-H bonds. The presence of too much cationic Pt results in more C²⁺ product with a decrease in the CH₄ conversion rate due to the reduced charge-carrier separation efficiency.

Oral Lecture: Magnetic Properties and Exchange Interaction of Ce/La Substituted Nanocrystalline NdFeB Alloys as a Function of Temperature Prepared by Melt-Spinning Technique

Muzaffar Hussain

Chairman, Department of Physics, Air University Islamabad, Pakistan

Abstract

The effects of La and Ce substitutions for Nd on the magnetic properties and intergrain exchange coupling interaction of nanocrystalline $(\text{Nd}_{1-x}\text{M}_x)\text{yFe}_{94-y}\text{B}_6$, ($\text{M}=\text{La}$ and Ce ; $y=12$; $x=0-0.4$) alloys have been studied and reported in order to improve room temperature and elevated temperature magnetic properties and reduce the rare earth content for NdFeB based alloys. Optimum magnetic properties such as remnant magnetization M_r , maximum energy product $(BH)_{\text{max}}$ and coercivity H_c up to 104 emu/g, 151 kJ/m³ and 9.0 kOe respectively have been obtained for direct quenched melt-spun single phase $(\text{Nd}_{0.95}\text{La}_{0.05})_{12}\text{Fe}_{82}\text{B}$ alloy. The fall in M_r for La/Ce substituted alloys is ascribed to the decrease in saturation magnetization. An unusual increase in H_c for 5% La substituted single phase alloy is speculated to the change in microstructure and magnetic phase separation. Elevated temperature behavior in the temperature range of 300 to 400K was studied for single phase alloys. The elevated magnetic properties with La substitution for Nd are higher compared to Ce substitution at 400 K. The analysis of remanence ratio and recoil loops reveal that La substituted alloys exhibit strong ferromagnetic exchange coupling than Ce substituted alloys due to the increase of exchange length and refine microstructure by La substitution. The present outcomes indicate that partial substitution of Nd by La or Ce leads to numerous change behaviors for magnetic properties at room temperature, elevated temperature and inter-grain coupling.

Oral Lecture: Various High-Efficiency Front TCO film Techniques for Silicon Solar cells

Shahzada Qamar Hussain

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Abstract

Front transparent conductive oxide (TCO) films play a vital role in silicon based thin film solar cells (TFSCs) due to their high transparency, conductivity and excellent light scattering properties. We report various front TCO films techniques for an enhancement in efficiency of silicon solar cells. Maskless large area randomly textured glass surfaces with various haze ratios were prepared by well controlling the ratio of buffered hydrofluoric acid (BHF) and sulfuric acid (H_2SO_4). Inverted hemisphere textured (IHT) glass surface morphologies with high transmittance and variable haze ratio were prepared by wet chemical etching. It was observed that haze ratio of textured glass was dependent on feature size, etching depth and rms roughness. Multi-textured aluminum-doped zinc oxide (AZO) films were deposited on micro-featured textured glass (random and periodic) surface morphologies and showed high transmittance and haze ratio in visible-NIR wavelength region. a-Si TFSCs deposited on randomly textured glass showed short circuit current density (J_{sc}) = 16.68 mA/cm² with an efficiency of 9.79%. An efficiency of 9.61% with J_{sc} of 16.55 mA/cm² was shown by a-Si TFSCs deposited on the periodic IHT glass superstrate. We will also provide advantage TCO films having high mobility and low carrier concentration for Silicon heterojunction. At the end, we have discussed the challenges and future of solar energy for Pakistan.

Oral Lecture: Facile Functionalization of Green Nanomaterial in Sustainable Energy and Environment

Rooh Ullah

Assistant Professor, University of Turbat, Balochistan, Pakistan

Abstract

Micro fibre alumina was synthesized using thermal urea precipitation technique and applied as support for the nano-sized ZnO precursor. The facile functionalization of nano sized ZnO in reactive adsorption desulfurization (RADS) performance and effect of diffusion rate in the desulfurization process were compared with commercially prepared alumina used as support for ZnO and Ni precursors. Higher breakthrough desulfurization activity and sulfur adsorption capacity were concluded that strongly depends on the diffusion rate of molecules, homogenous nano-sized ZnO dispersion and degree of active oxides interaction with support. Results shows that Ni/ZnO-Al₂O₃-fibre adsorbent achieved highest breakthrough sulfur removal (10 ppm) up to 31.2 mL and 94 mg S/g sulfur adsorption capacity. Whereas Ni/ZnO-Al₂O₃-Com reveals compromised desulfurization performance of 1741 ppm conversion dealing with 31.2 mL of feed accountable for the 39 mg S/g accumulative sulfur capacity. Detailed characterization results conclude that higher external diffusion of reactant molecules within the cross cross micro-fibre, nano-sized ZnO particles and their lower irreversible oxides interactions (IOI) may be the reasons for superior RADS performance of Ni/ZnO-Al₂O₃-fibre adsorbent.

Oral Lecture: Fabrication of Nano-porous Anodic Aluminium Oxide (AAO) by varying Anodization Parameters for Energy Applications

Danish Tahir, Asim Iltaf, Syed Irfan Raies

School of Chemical and Materials Engineering

National University of Sciences and Technology

Islamabad, Pakistan

Abstract

To produce close-packed Nano-pores using anodization process in aluminum foil by varying different process parameters of anodization process i.e. time of anodization, type of electrolyte being used, the temperature of the electrolyte, purity of aluminum foil and voltage being used. Prepared nano-porous aluminum foil can be used for the preparation of nanodots, nanorods which will then be used in fuel cells and other semi-conductors. The anodized aluminum surface which is also called anodic aluminum oxide can be used to grow liquid crystal molecules in those Nano-pores and use the orientation of liquid crystal for bio-sensing applications.

Oral Lecture: Manganese Oxide-based Hybrid Electrodes for Supercapacitor Applications

Zaeem Ur Rehman, Mohsin Ali Raza, Uzair Naveed, Aoun Husnain, Muhammad Faheem Maqsood

Department of Metallurgy & Materials Engineering, University of the Punjab, Lahore, Pakistan

Objective:

This research work aims to synthesize MnO₂-based hybrid electrodes for supercapacitor applications. Hybrids of MnO₂ with different carbon nanomaterials like graphene oxide, reduced graphene oxide (rGO), carbon nanotubes, were developed to study the effect of these materials on specific capacitance (SC) of MnO₂.

Method:

MnO₂ was synthesized by simple air calcination method at 200 °C. Calcination at this temperature resulted in an amorphous structure of MnO₂. Hybrid electrodes were developed by coating active material on Ni foam substrate using vacuum centrifuge mixer.

Results:

Characterization of the composite electrodes was carried out by X-ray diffraction and scanning electron microscopy. Electrochemical characterization of electrodes was carried out by cyclic voltammetry (CV), galvanostatic charge discharge (GCD) and electrochemical impedance spectroscopy (EIS) in 3 M KOH. CV analysis of the MnO₂ electrodes showed maximum capacitance of 176 F/g at 1 mVs⁻¹. Furthermore, MnO₂-CNTs composite with 10 wt.% CNTs showed enhanced capacitance of 315 F/g at 1 mVs⁻¹ among all other composite electrodes.

Conclusion:

10 wt.% CNTs increased SC of MnO₂ by 48%. CV analysis showed 86% charge retention at 50 mV/s for 1000 cycles. EIS analysis showed minimum charge transfer resistance at the electrode surface.

Oral lecture: Bioelectrochemical Conversion of CO₂ into Biofuels and Oily Wastewater Treatment

Farzeen Sheikh^a, Farhat Yasmeen^{a*}, Humayun Ajaz^a, Aqsa Ahmed^a, Iftikhar Ahmed^{b*}, Abdul Ghaffar^a, Hamid Raza^a

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^b Energy Research Centre, COMSATS University Isb., Lhr Campus

Abstract

Decrement in natural resources and increased environmental pollution has heightened up the demand for the production of fuels i.e. biologically synthesized, renewable in operation, with the least possible energy and chemical consumption. Electrocoagulation, a process that has been employed for the production and then conversion of CO₂ into alcohols, carboxylic acids and somewhat esters i.e. valuable energy producing biofuels. The source of CO₂ that has been utilized was synthetic oily wastewater, in order to get it converted into long chain hydrocarbons also, as those biofuels are considerably more these days. Aluminium was used as a sacrificial anode for the generation of coagulants naturally into the electrokinetic system. The experimental design was established using stainless steel and aluminium electrodes along with the recyclization of used engine oil so as to reduce the cause of oil spills and refineries pollution. Clean water was extracted after physical and electrochemical treatment given to the wastewater with 89% removal of COD, 64% reduction in the size of unwanted and hazardous flocs. The production of carboxylic acid with long chains has been investigated prior by the help of FT-IR of the sludge and later confirmed by the results of GC-MS. Linolenic esters in organic phase and acids of that group in the polar phase were reported. Cost effective design of experiment and production of precursors of energy and electricity, was the chief objective of this scrutiny. Application in fuel and energy market with better oil spill management is expected in future through this hybrid technique.



Poster Presentations

P-01**Fabrication of Graphene and its Nano-derivatives by Highly Efficient Route.**

**Muhammad Omer Farooq¹, Awais Ikram^{1,2}, Saif Haider Kiyani¹,
Sarmad Feroze³, Fazal A. Khalid^{1,3}.**

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³University of Engineering and Technology Lahore, Pakistan.

Abstract

In this research work we present an exceptionally efficient method to fabricate graphene for commercial scaling. Utilizing improvements in Modified Hummer's method we were able to synthesize good quality graphene considerably quicker by reducing the oxidation time with the aid of 9:1 ratio $\text{H}_2\text{SO}_4/\text{H}_3\text{PO}_4$ and KMnO_4 excluding NaNO_3 . This method requires cheap commercial grade graphite powder which also makes it economical alternative for producing large mass of graphene. Characterization of graphene was performed using Atomic Force Microscope, Raman spectroscopy, Scanning Electron Microscope and Energy Dispersive Spectroscopy. By controlling the processing parameters, chemical conversion of graphite to graphite oxide can be achieved effectively with distinct change in appearance from black to greenish brown and subsequently yellowish which marks existence of hydrophilic Graphite Oxide. This oxide can be exfoliated into nanometer sheets of graphene oxide by ultrasonication, magnetic stirring and thermal exfoliation. Defect peaks were evident in Magnetic Exfoliation, whereby ultrasonication proved to be the most useful asset in exfoliation to pristine graphene nanosheets. Processing time was significantly reduced from days to matter of few hours utilizing improvements in current practices in graphene production. Graphene produced was hydrophobic and grayish flake like

P-02**Electrical and Thermo Mechanical Properties of Poly (vinyl chloride) Reinforced with Carbon Nanotubes (CNTs)****Danish Tahir**

*School of Chemical and Materials Engineering
National University of Sciences and Technology
Islamabad, Pakistan*

Abstract

Poly vinyl chloride (PVC) with variable concentration of carbon nanotubes (CNTs) was synthesized to check the dependence of CNTs on the polymer properties and how this nano reinforcement affects its thermal and electrical properties. Concentration of CNTs is varied from 0.01% to 1 wt.%. Four probe electrical conductivity tests are used to examine the electrical behavior of the nanocomposite. CNTs insertion inside PVC affect its thermal properties which are explored by the means of thermo gravimetric analysis (TGA) whereas change in mechanical properties with variation in temperature also studied by thermo mechanical analysis (TMA). Experimental values obtained from these tests were then used to study the behavior of virgin PVC and effect of increasing CNTs concentration in nanocomposite.

P-03**Energy Efficient Building Using Building Modelling Techniques****Omar Saleem¹, Safeer Abbas², Saman Shahid^{1*}, Shahid Ali¹***¹ Department of Civil Engineering and Department of Sciences & Humanities, National University of Computer & Emerging Sciences (NUCES), FAST Lahore Campus, Pakistan**² Department of Civil Engineering, University of Engineering & technology (UET), Lahore, Pakistan***Abstract**

The construction has exponentially increased with increase in population causing pollution and greenhouse gasses. World is shifting towards Green Building Designs, but they are costly. The Energy Efficient Buildings helps recover extra cost initially invested on a structure by reducing energy consumption of a building by careful design parameters. Architecture Engineering and Construction (AEC) decisions can be precisely integrated such that a Green Building costs no more than a standard building. Overall goal for the research was to investigate the effectiveness of the energy performance tools for the energy analysis of the buildings. The research included three buildings to be analysed in the software programs that incorporate the green elements from US LEED and ASHRAE guidelines. We studied the material effects with various design alternatives on the total energy consumption of the building using Revit and Insight and achieve the best design alternative for all three scenarios. We determined the effect of using different materials, energy efficient and water efficient devices and independent energy producers in the selected alternatives on energy efficiency and compare initial and life cycle costs for all three scenarios. We discussed the effectiveness of Building Information Modelling technique capacity to handle the Life Cycle Cost Analysis (LCCA) and energy efficiency using Building Energy Performance Simulations in Pakistan.

P-04**Environmental Sustainability Via Renewable Resources****Sadia Naz¹, Maliha Uroos¹, Nawshad Muhammad²***¹Institute of Chemistry, University of the Punjab, 54000, Lahore, Pakistan.**²Interdisciplinary Research Centre in Biomedical Materials (IRCBM) COMSATS Institute of Information Technology, 54600, Lahore, Pakistan.***Abstract**

Production of 'Bioenergy' is the most critical demand in today's world threatening energy crisis. Utilization of renewable resources is the most challenging research in this regard. Biomass waste material is the only renewable, abundant and carbon-economic material for bioenergy production. We have introduced a green, eco-safe and highly economic ionic liquid [C₄C₁P_y]Cl as a solvent for effective biomass conversion. 28% Cellulosic dissolution and 78 % sugars formation was observed at optimum conditions. Various analytical methods like FTIR, ¹HNMR, UV, SEM, TGA, XRD were performed to characterize synthesized green solvents as well as cellulose and sugar products obtained after processing of renewable feedstock in ionic liquid.

P-05**Synthesis, Characterization & Applications of TiO₂ Hollow Nanostructures by Hydrothermal Route for Commercial Scale Up****Muhammad Omer Farooq¹, Awais Ikram^{1,2}, Fazal A. Khalid^{1,3}**¹*Faculty of Materials and Chemical Engineering, Ghulam Ishaq Khan Institute of Engineering Science & Technology, Pakistan, (23404).*²*Department of Nanostructured Materials K7 Nano, Jozef Stefan Institute, Ljubljana, Slovenia, (1000).*³*Vice Chancellor, University of Engineering and Technology Lahore, Pakistan.***Abstract**

This study presents simple route to synthesize Titanium Dioxide Nanotubes (TNT) using Low Temperature Alkaline Leaching (Hydrothermal), which is easily reproducible. We have used three different hydrothermal methods to develop Nanotubular structures of Titania utilizing powder Nano Rutile Mineral (APS 50 nm) which has been reported much less in similar studies previously. Characterization was accomplished with tools include XRD, SEM and EDS. Length of tubes grown can continue in micrometer range with tunable diameters through Hydrothermal Processing. Diameter of our fabricated TNTs was observed in nanoscale range (65-200 nm for discontinuous TNTs at nucleation sites while 200-400 nm for individual continuous nanotubes), for which lengths continue in order of hundreds of nanometers to few microns (>1000 nm on average). Controlling processing parameters can help develop range of different nanostructures like nanotubes, nanowires, nanorods, nanoribbons etc. with same hydrothermal approach. The method is good to scale up multiwall Titania Nanotubes for commercial applications in photoactive devices, photosensors, gas sensors and storage devices (H₂, O₂) and dye sensitized solar cells.

P-06**New Energy Conversion Device Using SiC as Potential Semiconductor****Asif Hassan Raza***Department of Physics, COMSAST University Islamabad, Lahore Campus***Abstract**

Silicon carbide is well known because of semiconductor and excellent potential in energy devices due to its better electrical and mechanical properties. It has maximum avalanche breakdown, best thermal conduction, and maximum velocity of electron charge carrier, it has many applications due to its non-oxide behavior, high melting point, rigorous firmness, high oxidation resistance, rust resistance, and mechanical strength. It has charming characteristics. These complimentary characteristics make SiC an auspicious material that used in electrical devices. SiC crystal exists in a lot of various crystal structures. The most attractive of them is cubic silicon carbide (3C-SiC). The main advantage of 3C-SiC is that it has high electron mobility and phonon scattering.

In this paper, silicon carbide is prepared using hydrothermal method. The Si-C is used as anode material for fuel cell and studied the performance of the cell at temperature range (200-500 °C). The conductivity of the material is also obtained at this temperature. The detailed analysis and phenomenon behind the device will be studied using electrochemical analysis and other material characterization techniques, XRD, SEM, and UV-Vis, to study the composition, structure, surface morphology of the material, the band gap and thermal analysis respectively has been studied and analyze to support the fuel cell performance.

P-07**Integrated Plastic Solid Waste Management (ISWM) System Based on 3R Principle and Resource Conservation and GHG Emissions**

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Abstract

Plastic pollution is increasing day by day and demand of producing a successful remedy to counter this pollution has been increased also. This research was conducted to reduce plastic solid waste and greenhouse gases emission by using 3R principle which involves reducing, reusing and recycling techniques to reduce the plastic waste. In first stage solid waste was collected while second stage involves recycling of polymer which is in higher quantity in the waste i.e. polyethylene terephthalate (PET). Recycling process was done by shredding, cleaning and injection molding whereas certain properties were enhanced by blending with additives such as polypropylene (PP) or polyethylene (PE). Characterization techniques includes differential scanning calorimetry (DSC), scanning electron microscopy (SEM) and tensile testing. PET/PP with 80/20 ratio showed excellent morphology and mechanical properties. Percentage crystallinity of 82.2% was observed in high density polyethylene (HDPE) whereas PET showed a minimum crystallinity of 30.9%.

P-08**Bismuth doped Gd-Ceria Electrolyte for Solid Oxide Fuel Cell**

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Abstract

Bismuth substituted Gd-ceria is prepared by a simplified sol gel method. Four sample with composition $\text{Ce}_{0.75} \text{Gd}_{(0.25-x)} \text{Bi}_x \text{O}_{(2-\delta)}$ ($x=0.0, 0.05, 0.10, 0.15$) were prepared to check the effects on conductivity. The structural analysis through x-ray diffraction (XRD), morphology analysis by scanning electron microscopy (SEM) and electrical measurements including DC conductivity, dielectric constant, dielectric loss tangent, AC conductivity and impedance were carried out to characterize these materials for electrolyte applications. An enhancement in electrical conductivity is observed by substitution of Bi in sample. Therefore, Gd-ceria substituted with Bi appears to be a good candidate for electrolyte applications.

P-09**Metal Sulfides for Energy storage devices****Muhammad Inam Khan, Yasir Usman***Department of Physics, COMSATS University Islamabad, Lahore
Campus, Pakistan***Objective:**

Global warming, climate change and shortage of fossil fuels demands for the new sustainable and renewable energy resources. As we know that the sun does not shine at night and winds are not controlled by us therefore there is a great need for energy storage systems And here the batteries and electrochemical capacitors (ECs) play a very important role in our daily life However we still need to improve their efficiency, performance and quality.

Methods:

The composite was prepared by a simple precipitation method. For this Zinc acetate and tin chloride were used as the precursor. Finally, the precipitates were dried and used for further characterization. X-ray diffraction (XRD) and scanning electron microscopy (SEM) were utilized for characterization. XRD analysis verified presence of $\text{ZnSn}(\text{OH})_6$ structure. While SEM analysis showed that composites have cubical morphology.

Results:

Electrochemical characterization was carried out by cyclic voltammetry (CV) and galvanostatic charge discharge (GCD). The CV results showed that the prepared composite have good oxidation - reduction peaks. Moreover, the composite was then mixed with a cellulosic fiber and made flexible sheets of it for flexible batteries.

P-10**Synthesis and Characterization of Cu Based Ternary Metal Oxide for Photocatalytic Hydrogen Production****Farooq Ahmad, Ahmad Kaleem Qureshi, Muhammad Babar Taj, Muhammad Imran****Department of Chemistry, Baghdad-UI-Jadeed Campus, The Islamia University of Bahawalpur, Bahawalpur 63100, Pakistan***Abstract**

Hydrogen production through photocatalytic water splitting is a sustainable technology for the clean solar energy conversion to emerge in recent years. In the present research work, we have developed a rapid and facile precipitation method for the fabrication of ternary metal oxide (Cu_2NiO_4) photocatalyst using different copper precursors in the presence of ammonia as capping and stabilizing agent. Moreover, in order to investigate the size and morphology, the photocatalyst was thermally treated at different temperature. The synthesized catalyst was characterized by using various analytical and imaging techniques such as ultraviolet- visible (UV-Vis), Fourier transform infrared (FT-IR), powder X-ray diffraction spectroscopy (PXRD) scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDX). The photoactivity of the synthesized catalyst was evaluated by hydrogen production from photocatalytic water splitting and the results revealed that the hydrogen evolution rate was $29 \mu\text{mol g}^{-1}\text{h}^{-1}$ after 5 h cycle. The results indicated that the prepared photocatalyst has potential applications in photocatalytic hydrogen production.

P-11**NiCoAl Mixed Metal Oxides-Based Electrodes for Arsenic Removal from Groundwater by Capacitive Deionization**

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Hamza Butt ^b, Asma Saeed ^b**

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Objective:

The scarcity of clean drinking water resources has become one of the most important issue worldwide. According to the International Agency for Research on Cancer (IARC) arsenic (As) is considered as carcinogenic to humans. Therefore, a maximum allowable limit of 10 parts per billion (ppb) was recommended by the World Health Organization. In this research, a novel method of As removal from water, capacitive deionization (CDI) which is based on electrosorption has been presented.

Methods:

The ternary component NiCoAl mixed metal oxides (MMOs) 3D structure was prepared as electrode on a nickel foam substrate. These electrodes were prepared by a simple hydrothermal reaction with optimal Ni/Co/Al ratio (1.5:1.5:1). Hydrothermal reaction was carried out at 180 oC for 10 hours followed by calcination at 500 oC for 4 hours. Synthesized MMOs were characterized by x-ray diffraction (XRD) and scanning electron microscopy (SEM). XRD analysis verified presence of NiCoAl MMO structure. SEM analysis showed that MMOs have particulate morphology.

Results:

Electrochemical characterization was carried out by cyclic voltammetry (CV). CV analysis showed that MMO-based electrode showed maximum specific capacitance (Cs) of 260 F/g at 1 mV/s in 3M KOH. Electrosorption experiments were carried out in batch type CDI cell. Effect of time and stock solution concentration was studied on electrosorption capacity of electrodes.

P-12**Catalytic Degradation of Low Density Polyethylene Using Silica Supported Vanadium Substituted Silicotungstate****Muhammad Junaid¹, Asma Tufail Shah², Madeeha Batool^{1*}**¹*University of The Punjab, Lahore*²*IRCBM, COMSATS University Islamabad, Lahore Campus, Pakistan***Objective:**

Use of Multi-transition metal oxides as economic and environmentally friendly catalysts for the degradation of polyethylene

Method:

In this study, vanadium substituted silicotungstate (VSiW₁₂O₄₀) was supported on the surface of SBA-16 and MCM-41. FTIR, TGA and XRD were used to characterize the supported catalysts. These supported catalysts were employed for the catalytic cracking of low density polyethylene.

Results:

Results revealed that MCM-41 supported vanadium substituted silicotungstate (VSiW₁₂O₄₀) showed better yield of oil and less degradation temperature among the synthesized catalysts. Furthermore, GC/MS was used to investigate the number of useful hydrocarbons produced after catalytic cracking of polyethylene.

Conclusion:

Synthesized supported catalysts are quite efficient for the degradation of low-density polyethylene (LDPE)

P-13**Amine-based CO₂ Capture for NGCC Power Plant with Selective Exhaust Gas Recirculation****Yamina Qureshi, Usman Ali***Department of Chemical Engineering, University of Engineering and Technology, G.T. Rd, Lahore 54890, Pakistan***Background:**

Fossil fuels play a significant role in increasing energy demand, which is the major source of anthropogenic CO₂ emissions. CO₂ is one of the main greenhouse gases and have an impact on global climate change, therefore, carbon capture and storage is becoming essential.

Objective

The study is conducted for modelling and simulation of NGCC power plant and CO₂ capture plant with SEGR (series, parallel and hybrid) using Aspen Plus.

Method:

A CCGT plant with SEGR in series, parallel, and hybrid configuration to the PCC system is exploited using Aspen plus. Performance parameters are analyzed to optimize the SEGR ratio to maximize the fraction of CO₂ concentration and to reduce specific reboiler duty.

Results:

For hybrid configuration, a CO₂ concentration in flue gas is enhanced to 18 vol.%, and specific reboiler duty reduces to 3.32 MJ/kg CO₂. SEGR in parallel increases the CO₂ concentration by 14 vol.% at the inlet of the PCC system operating at 70% SEGR ratio and reduces the specific reboiler duty to 3.42 MJ/kg CO₂. For SEGR in series, a CO₂ concentration of 13 vol.% is attained and reduces the reboiler duty to 3.56 MJ/kg CO₂.

Conclusion:

The integration of NGCC plant coupled, with amine capture plant, in Aspen plus is analyzed. The SEGR process operated in series, parallel and hybrid configuration reduces 5-7% specific reboiler duty and increase the CO₂ concentration in the exhaust flue gas of CCGT power plant by maintaining 19 vol.% oxygen level in the combustor.

P-14**Nano Structured Transition Metal Oxide Catalyst for Water Splitting****Ramsha Khan, Muhammad Taqi Mehran***School of Chemical and Material Engineering, National University of Science and Technology, Islamabad.***Objectives:**

Perovskite has proven to be an effective field of research in heterogenous catalysis based on electrocatalytic water splitting process. Here in, we present a novel idea of combining a hybrid Perovskite, having exceptional electronic and magnetic properties with 2D transition metal, MXene. The objective is to prepare an inexpensive catalyst with activity compareable to state-of-the-art catalyst Platinum.

Method:

The Perovskites were prepared by Sol gel method while MXene was prepared by using Hydrofluoric acid. The composite was prepared via ex-situ process with diverse $\text{La}_{0.4}\text{Sr}_{0.4}\text{Ti}_{0.9}\text{Ni}_{0.1}$ and $\text{L}_{0.6}\text{S}_{0.4}\text{C}_{0.2}\text{F}_{0.8}$, combinations with $\text{Ti}_3\text{C}_2\text{Tx}$.

Results and Conclusion:

The composites were prepared in three ratio's and were compared correspondingly. LSTN:MXene(1:2) and LSCF:MXene(1:1) had shown the highest activity as a bifunctional catalyst for Oxygen evolution and Hydrogen evolution reaction. The composite electrocatalyst was characterized by using SEM, XRD and BET analysis as well as electrochemical testing such as cyclic voltammetry, EIS. The high surface area nanostructured composite exhibited very low Tafel slope along with low overpotential and high current density values. The process enhanced the electrochemical properties of Perovskite, also filling the voids in stability. This new idea of combining 2D materials with Perovskite opens up a way to develop more advanced materials for various energy applications.

P-15**Synthesis and Structural Characterization of silver(I)
Complexes and Coordination Polymer****Naila Yamin, Muhammad Altaf, Raja Shahid Ashraf***Department of Chemistry, Government College University Lahore,
Pakistan***Abstract**

The emergence of microbe's resistant antibiotics against bacterial infections is a worldwide problem that provoked the development of novel antimicrobial agents. Silver metal and silver salts has been utilized as antimicrobial agents for thousands of years. Due to its antimicrobial activity, silver(I) complexes provide a versatile platform for drug design and are captivating parts of bioinorganic chemistry. Mixed ligand silver complexes have been reported in the literature and shown promising activity against microorganisms. Here in, we synthesized, characterized a series of three new silver(I) complexes that contain bisphosphine and dithiocarbamate (DTC) ligands. The structures of new complexes were characterized using spectroscopic and analytical techniques. Single crystal studies revealed that the geometry of two complexes is binuclear and one complex is one-dimensional (1D) polymer, respectively.

P-16**Synthesis and Characterization of Bimetallic Composites of Ti/Ni for Wastewater Treatment.****Nabia Sohail***Department of Chemistry, Government College University Lahore,
Pakistan***Abstract**

This research work has carried out to investigate cheap, cost effective, and simple in terms of its methods, stable synthesis of bimetallic Ti/Ni composite and high adsorption capacity strategy for the removal of azo dyes. That is why new modified Ti/Ni composite supported on functional bentonite clay was synthesized followed by liquid phase reduction method. The synthesis of these NPs was confirmed by different characterization techniques like Particle size analyzer, UV-Vis, SEM, EDX and XRD. The diameter of these NPS was found below 50 nm. The affinity of Ti/Ni-Bentonite NPs towards azo dyes was checked and results showed that 27.2% MO dye, 66% MB dye and 77% MG dye removal was achieved within 120 minutes. The research work examined the difference between the % removal efficiency of Ti/Ni and Ti/Ni-Bentonite and found that 23% and 77% removal of MG dye was achieved respectively. The optimal conditions for parameters were observed as; at pH 8, 68% and within the time interval of 120 minutes 77% removal of MG dye, at 40 mg/L, 91% removal of MG dye and at 3 ml of 50 wt.% solution, 95% methyl green dye from the solution was achieved. The results provide evident that new modified bimetallic Ti/Ni-Bentonite catalyst was an efficient and cost-effective method for the removal of azo dyes.

P-17**Synthesis of Nanocomposite for Water Splitting Through Photocatalysis****Muhammad Mudassir Hassan, Muhammad Nasir****IRCBM, COMSATS University Islamabad, Lahore Campus***Abstract**

Depletion of fossil fuels and the problems and hazards caused by their combustion are creating wide environmental issues for the ecosystem. Therefore, in order to cope up with the increasing energy demands in the fast growing world, looking for new alternative and sustainable energy resources is highly needed. Finding out clean energy resources could also decrease the greenhouse emissions and harmful. Hydrogen is considered as clean and renewable energy for our future energy requirements. In order to find out the ways to acquire hydrogen, photocatalysis is the most efficient and cheap method. Therefore, a series of $\text{WO}_3/\text{g-C}_3\text{N}_4$ composites with different WO_3 contents were prepared via a facile in-situ method and showed notably enhanced visible-light-driven photocatalytic H_2 -evolution activities. The prepared photocatalyst showed much higher activity than the pristine $\text{g-C}_3\text{N}_4$. It has been successfully optimized that the Z-scheme system constructed by WO_3 and $\text{g-C}_3\text{N}_4$ have effectively reduced the recombination of photogenerated charge carriers in pristine $\text{g-C}_3\text{N}_4$. The photocatalytic activity of the photocatalysts were evaluated by degradation of methylene blue (MB) and Methyl Orange (MO) dye under visible light. The results indicated that the $\text{WO}_3/\text{g-C}_3\text{N}_4$ composite photocatalysts showed higher photocatalytic activity than both the pure WO_3 and pure $\text{g-C}_3\text{N}_4$. Moreover, pore size and surface areas of the composites were gradually decreased by introducing the WO_3 into $\text{g-C}_3\text{N}_4$ via in-situ method. The remarkably increased performance of $\text{WO}_3/\text{g-C}_3\text{N}_4$ was mainly attributed to the synergistic effect between the interface of WO_3 and $\text{g-C}_3\text{N}_4$, including enhanced optical absorption in the visible region, and the suitable band positions of $\text{WO}_3/\text{g-C}_3\text{N}_4$ composites.



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