BOOK OF ABSTRACTS

INTERNATIONAL CONFERENCE ON MATERIALS FOR ENERGY ENVIRONMENT AND HEALTHCARE

MEEHCON '24

20,21 DEC 2024

Department of Materials Science and Engineering
National Institute of Technology Calicut

WELCOME NOTE FROM THE ORGANISERS

Dear Participants,

It is with great pleasure that we welcome you to the 2nd Conference on Materials in Energy, Environment, and Healthcare, organized by the Department of Materials Science and Engineering (MSED). Following the success of the inaugural conference held on December 27–28, 2019, we are thrilled to host this second edition.

The primary goal of this conference is to provide a dynamic platform for sharing ideas and fostering collaborations in the rapidly evolving fields of materials science, particularly in energy, environment, and healthcare. The overwhelming response from participants across academia, research, and industry reflects the importance of these areas in shaping a sustainable future. The two-day technical program is designed to inspire and engage participants with a rich mix of keynote addresses, invited lectures, parallel sessions, and oral/poster presentations.

- Day 1 features 6 keynote sessions delivered by eminent speakers, followed by 8 invited lectures focusing on distinct thematic areas.
- Day 2 includes 4 keynote sessions and 9 invited lectures.

Altogether, the conference comprises an impressive list of oral and poster presentations, showcasing a broad spectrum of cutting-edge research. To recognize excellence in research communication, Best Oral and Poster Presentation Awards are sponsored by the Royal Society of Chemistry (RSC) American Chemical Society (ACS) respectively.

We extend our heartfelt gratitude to the speakers, participants and sponsors for their invaluable contributions in making this event a grand success. We hope this conference provides an enriching experience, sparking new ideas and collaborations that advance the frontiers of materials science.

Once again, welcome to the conference, and we wish you two days of engaging discussions and fruitful interactions.

Warm regards,
Organizing Committee, MEEHCON'24

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AWARDS AND PRIZES

The best oral and poster presentations in each track will be recognized with best paper awards. The prizes for posters are sponsored by **ACS International Ltd.** The winners will get certificates from,

- **ACS Applied Nano Materials**
- **ACS Applied Energy Materials**
- **ACS Applied Electronic Materials**
- **ACS Sustainable Resource Management**
- **ACS Omega**

The best oral presentations will be awarded gift certificates provided by **Royal Society of Chemistry (RSC).**

ABOUT MSED

The Department of Materials Science and Engineering (Formerly School of Nano Science and Technology) at National Institute of Technology Calicut offers programs at the Bachelors, Master's and Doctoral levels, in various academic streams related to Materials Science and Engineering. The department also houses sponsored research projects from various funding agencies. The faculty, students and research scholars are involved in dedicated learning and research to explore, understand and improve materials and processes from a fundamental perspective. They pursue academic research leading to the mission to introduce new functionalities into existing materials, and to tailor-make materials with exceptional qualities, which are the two major goals of Materials Science and Engineering. The varied interests of the department include study of nanoscale physical phenomena, materials for sustainable energy solutions, nanodevices, nanomaterials and composites, biosensors, targeted drug delivery systems, bio-implants, experimental research in nanoscale flow and heat transfer, optical measurements, combustion and nanoparticle fuel additives, synthesis of nanomaterials including carbon nanotubes, and discrete computational studies on nanoscale systems using molecular dynamics simulations. The department is equipped with various characterization techniques, such as a Scanning Electron Microscope, Fourier Transform Infrared Spectroscopy and Scanning Probe Microscope. Additionally, other instruments are available to support student projects. The department offers a four-semester Master of Technology program in Nanotechnology and a four-year Bachelor of Technology program in Materials Science and Engineering.

Scope of the MEEHCON'24

The integration of advanced materials into energy, environmental, and healthcare applications is a cornerstone for addressing global challenges and achieving sustainable development. This conference aims to explore cutting-edge research and innovations in materials science, focusing on their roles in energy generation, storage, and efficiency, as well as their impact on environmental sustainability and healthcare advancements.

In the energy sector, discussions will revolve around the development of novel materials for photovoltaic systems, hydrogen production and storage, fuel cells, batteries, and supercapacitors, all aimed at fostering clean and efficient energy solutions. Environmental applications will focus on materials designed for air and water purification, carbon capture and conversion, and waste management, addressing the urgent need for ecological preservation.

The healthcare domain will emphasize the transformative potential of materials in diagnostics, drug delivery systems, tissue engineering, and the development of implants and implantable devices. Emerging trends in biocompatible and multifunctional materials will also be a key focus.

This conference provides a platform for interdisciplinary collaboration, bringing together scientists, engineers, and industry experts to discuss the latest advancements and future directions in materials research for energy, environment, and healthcare.

CONTENTS

Multi-purpose Electron Microscope

Scientific / Metrology Instrument

JEM-F200

Smart design:

Design concept "Smart" focused on a user interface for intuitive operation.

Quad-Lens condenser system:

New illumination system to
independently control electron-beam intensity and convergence angle.

Advanced Scan system:

Incorporating a De-Scan system in the imaging lens system(optional)

Pico Stage Drive:

Field-of-view can smoothly move in steps of the "pm" order.

SPECPORTER™ (automatic holder insertion & retraction):

Enables smoother holder insertion & retraction by simply pushing a button.

Improved Cold FEG:

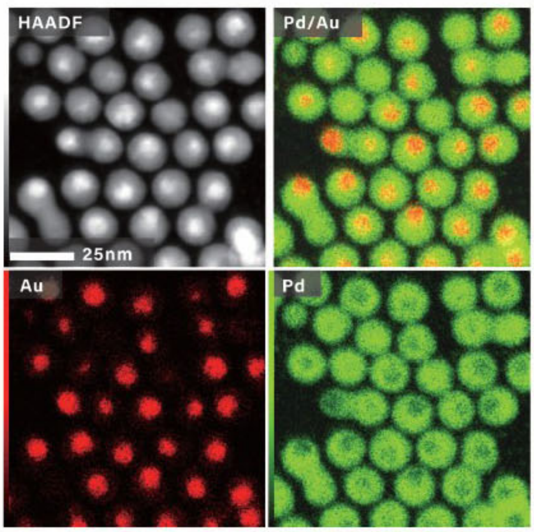
Cold field emission gun (Cold FEG: optional) producing a high-stability, high-brightness electron beam for high energy-resolution EELS.

Dual SDD:

Two large-solid angle, high-sensitivity silicon drift detectors (SDDs: optional) can simultaneously be installed

Environmental friendly:

Standard ECO mode system saves energy efficiently
when the microscope is not used.



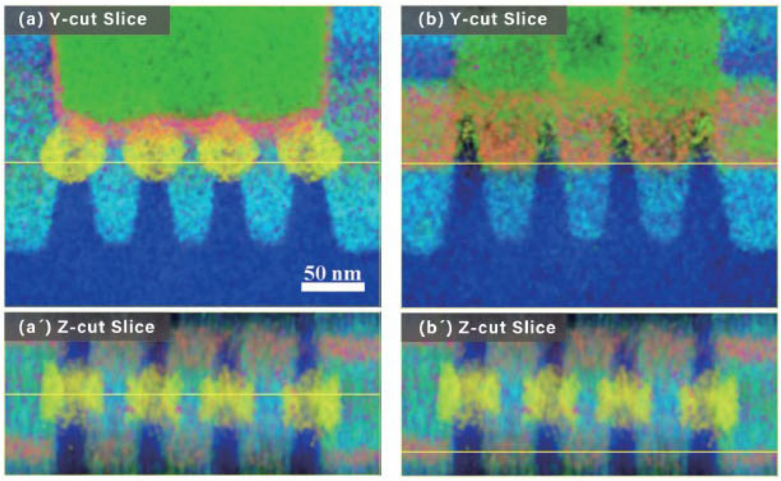
512 × 512 pixel, ~5 min

Data courtesy : Prof. A. I. Kirkland
Oxford University

Specimen courtesy : Dr. R. D. Tilley and Dr. Anna Henning
Victoria University of Wellington

Fig. 1. Elemental maps of core-shell structured catalyst particles

Since Dual SDD has high detection efficiency, you can rapidly acquire clear elemental distributions even from a catalyst specimen susceptible to electron-beam damage, as shown in Fig. 1 (Au core region and Pd shell region).



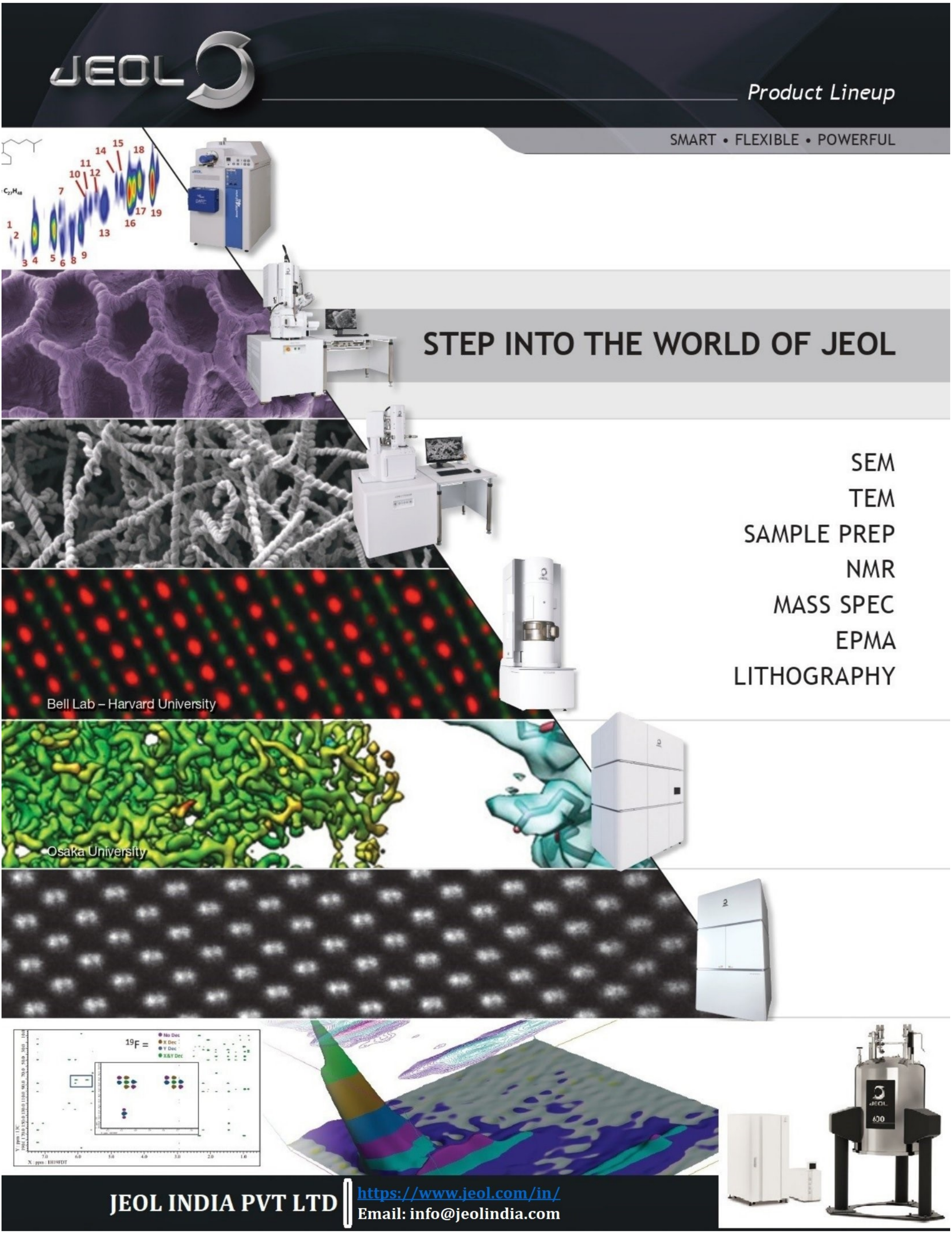
Reconstruction Technique: SIRT (Simultaneous Iterative Reconstruction Technique) *

* SIRT is an effective technique to reconstruct EDS tomography because the influence from missing wedge or noise is very small.

Fig. 2. 3D elemental maps of semiconductor specimen

Shorter acquisition time of Dual SDD enables 3D tilt-series elemental maps to be obtained from FinFET by EDS tomography. Fig. 2 shows detailed results.Y-cut and Z-cut slice maps extracted from 3D elemental maps of FinFET using EDS tomography are shown. (a) and (b) show elemental maps of the Y-cut slices at different positions indicated by a yellow line in the corresponding Z-cut maps below. The Z-cut slice is parallel to the wafer surface. Elemental information on the Si/Ge stressor and the Tri-Gate structure in the channel are confirmed.

JEOL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INVITED ABSTRACTS

Understanding Structural and Functional Properties of Materials using Advanced 4D-STEM Techniques

Prof. Christian Kübel
In Situ Electron Microscopy, Technical University Darmstadt
E-mail: christian.kuebel@kit.edu

ABSTRACT

Electron microscopy has seen tremendous developments over the last couple years providing unprecedented possibilities in materials characterization at the nanometre and atomic scale. With the high spatial resolution and high beam currents available in aberration corrected (S)TEM, highly sensitive detectors for imaging and spectroscopy and fast readout speeds, new microscopy methods have been established, which enable advanced insights into materials, their 2D/3D structure and chemistry as well as some of their functional properties. In particular, the recently developed 4D-STEM techniques are promising an improved understanding of both crystalline and amorphous materials. This provides an overview of the techniques and the information that can be obtained by transmission electron microscopy, focusing in particular on 4D-STEM techniques to correlate local structure description with local functional properties such as strain, magnetic and electric fields to understand complex nanomaterials. This also illustrates the capabilities looking at deformation and annealing of metallic glasses and polymer composites as examples for (partially) amorphous materials and grain boundaries in oxides used in solid electrolytes or as ferroelectrics.

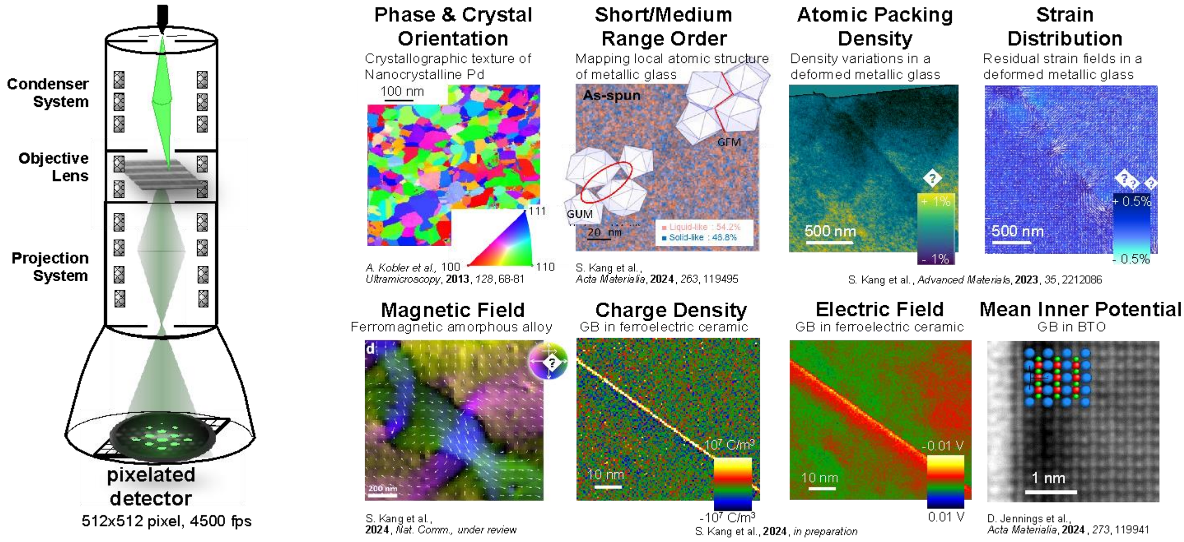

Figure 1: Illustration of the capabilities of 4D-STEM materials analysis.

Keywords: 4D-STEM; Aberration corrected STEM; Strain distribution; Phase and crystal orientation; Deformations.

References:

[1]X. Mu et al., *Ultramicroscopy*, 2016, *168*, 1-6; 10.1016/j.ultramic.2016.05.009.

[2] S. J. Kang et al, *Acta Materialia*, 2024, *263*, 119495; 10.1016/j.actamat.2023.119495.

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[4] X. Mu, A.A. Mazilkin, C. Sprau, A. Colsmann, C. Kübel, *Microscopy*, 2019, *68(4)*, 301-309; 10.1093/jmicro/dfz015.

[5] Z. Ding et al. *Advanced Energy Materials*, 2023, *13(48)*, 2302322; 10.1002/aenm.202302322.

Exploring the Role of Carbon Quantum Dots in Enhancing Plant Functions: Innovative Approaches and Future Prospects

Dr. Jaya Jacob

Scientist, Kerala State Council for Science Technology and Environment

Thiruvananthapuram, Kerala

E-mail: jaya.kscste@kerala.gov.in

ABSTRACT

As the global population continues to grow, the world is rapidly adopting a resource-intensive lifestyle. This shift, coupled with the harmful effects of pollution, climate change, and changes in land use, has raised significant concerns. India, ranked as the third-largest carbon emitter globally, is urged to reduce its carbon footprint by nearly 35% by 2030. However, reports indicate that CO_2 emissions due to pollution are expected to double over the next 30 years, exacerbating the challenges of climate change. To address these issues, transdisciplinary, holistic approaches focusing on the development of smart biological systems with improved solar energy conversion and enhanced CO_2 reduction potential are crucial. One promising approach is engineering plant functions using non-toxic green nanoparticles to improve photosynthesis. In this context, developing "super-powered plants" with enhanced photosynthetic activity is of paramount importance. These plants can harness the full solar spectrum, leading to improved efficiency and better performance. Plants with enhanced photosynthesis can not only help maintain a balance by providing oxygen-rich air but also absorb the rising CO_2 levels in the atmosphere. Carbon Quantum Dots (CQDs), zero-dimensional carbon nanoparticles, have shown potential in tuning plant spectral responses due to their unique optical properties. In a recent study, CQDs were biosynthesized through a hydrothermal method and characterized to possess spectroscopic and morphological features similar to those of chemically synthesized CQDs. The biosynthesized CQDs exhibited strong emission at a wavelength of 520 nm, with an optimal excitation at 400 nm. These non-toxic nanoparticles were then employed to engineer plant functions for improved photosynthesis. The biogenic CQDs were integrated into the model plant *Vigna radiata* to enhance both growth and photosynthetic efficiency. Plants treated with 0.02 mg/mL of CQDs recorded a maximum chlorophyll content of 10.6 mg/L, indicating improved photosynthetic capabilities. The results demonstrate the promising potential of CQDs in the development of nanobionic systems for efficient photosynthetic carbon reduction, offering a sustainable solution to address rising CO_2 levels and contribute to global environmental sustainability.

Keywords: Carbon quantum dots; Hydrothermal treatment; Mung beans Photosynthesis; Plant nanobionics.

Development of Tough and Porous Complex Architecture using Energy Efficient Sustainable Additive Manufacturing

Prof. Chandra Sekhar Tiwary

Department of Metallurgical and Materials Engineering, Indian Institute of Technology Kharagpur, Kharagpur 721302, India

E-mail: chandra.tiwary@metal.iitkgp.ac.in

ABSTRACT

High surface area porous ceramic architectures are widely employed as heterogeneous catalytic carriers due to their surface functionalities and thermal stability across a broad temperature range. Additive manufacturing via direct ink writing (DIW) offers an effective method to create intricate ceramic structures, which cannot be made by conventional techniques. The resolution limitations in DIW restrict the fabrication of structures with smaller feature sizes. Additionally, insufficient solid loading during ink preparation can compromise the mechanical properties of the printed structures. Increasing the solid loading often leads to higher viscosity, which in turn can adversely affect printability. The solid loading has been maximized and optimized rheology for printing of ceramic materials ink by reducing the particle size of the powder. This approach has led to improved printability and enhanced printing resolution. Despite having a lower relative density compared to solid structures, the mechanical properties of porous additive manufacturing structures were superior, showing enhancement in compressive strength over solid structures.

Keywords: Additive manufacturing; Direct ink writing; Ceramic materials; Boehmite; Catalytic carriers.

Hybrid Organic-Inorganic Functional Materials: A New Strategy of Material Design

Dr. Sachindra Nath Sarangi

Institute of Physics, Sainik School P.O, Bhubaneswar751005, India
E-mail: sachin@iopb.res.in

ABSTRACT

Designing new functional nanomaterials through organic-inorganic hybrids (OIH) creates low-dimensional systems with unique and advanced properties, unlocking significant potential across various applications. Nucleotides, the fundamental components of living organisms, serve as the building blocks for biological coenzymes and nucleic acids. Recently, there has been a growing interest among researchers in leveraging versatile biomolecules such as glucose, DNA, and proteins to develop OIH and regulate the functionality of nanomaterials. Their remarkable features-including structural diversity, multiple binding sites, self-assembly abilities, stability, biocompatibility, and chirality-make them very fascinating. Various methods for synthesizing low-dimensional systems and shaping their characteristics using oligonucleotide templates were studied. Furthermore, there are studies focused on nanobiosensors and quantum magnetism.

Keywords: Organic-inorganic hybrids; Biomolecules; Oligonucleotide templates; Nanobiosensors; Quantum magnetism.

References:

[1] S. N. Sarangi et. al. Journal of Biomedical Nanotechnology 11 (6), 988-996 (2015).
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Electrification of Ceramic Manufacturing

Devinder Yadav, Akash Kumar Jaiswal, Vikaskumar Mishra

Department of Metallurgical and Materials Engineering, Indian Institute of Technology Patna, Bihta, Patna 801106, India

E-mail: devinder@iitp.ac.in

ABSTRACT

Materials-discovery and rapid-processing with electric and magnetic fields is emerging as the next giant step in the science and technology of materials research. It began with microwave sintering in the nineteen eighties, followed soon thereafter by spark-plasma-sintering (SPS), followed by the development of "flash-sintering" in 2010 where extraordinary rates of reaction rates were achieved. The simplicity of flash sintering experiment where electric power is applied directly to the specimen, in open view, is a radical development. The specimen can be watched in-operando with a camera, the temperature measured with a pyrometer, and the electroluminescence spectrum characterized with a spectrometer, all in real time. Flash sintering is a process where the sample sinters in a few seconds at significantly lower furnace temperatures by application of electric field across the sample. The furnace temperature at which a specimen can be flash sintered, can be lowered by increasing the strength of the applied electric field. The lower temperature limit being the Debye temperature of the material. The constraint of sample geometry is overcome by the "touch-free" flash sintering method, where specimens of any geometry can be sintered since the electrodes are not in contact with the workpiece. Techno-economic analysis shows that the energy consumption during flash-based processes is far lower than that during conventional processing. The microstructure evolution, mechanical properties and phase evolution during flash-based processes for specific systems will be discussed in detail.

Keywords: Flash-sintering; Applied electric field; Debye temperature; Microstructure evolution; Ceramics.

Beyond Lithium-Ion: All-Solid-State Batteries

Prof. M. M. Shaijumon

School of Physics, Indian Institute of Science Education and Research Thiruvananthapuram, Vithura, Thiruvananthapuram 695551, Kerala, India

E-mail: shaiju@iisertvm.ac.in

ABSTRACT

Driven by technology advancements, the global demand for sustainable and efficient energy storage systems continues to grow, and the spotlight is on the development of next-generation batteries. The next generation of batteries is assured to revolutionize the field of energy storage technologies, with all-solid-state batteries (ASSBs) emerging as a promising alternative to conventional lithium-ion systems. Unlike traditional batteries that rely on liquid electrolytes, ASSBs use solid-state electrolytes, offering significant advantages in terms of safety, energy density, and stability. This talk will explore the cutting-edge developments in all-solid-state battery technology, addressing the key materials, design challenges, and the benefits over liquid-based counterparts. The talk will further highlight some of our recent efforts towards developing lithium- and sodium-based all-solid-state batteries, with a focus on electrode/electrolyte interface engineering.

Keywords: Energy storage; All-solid-state batteries; Electrode/electrolyte interface engineering.

Multifunctional nanocarriers as magic bullets for combinatorial therapy

T. S. Sampath Kumar

Medical Materials Laboratory

Department of Metallurgical & Materials Engineering

Indian Institute of Technology Madras, Chennai 600 036

Email: tssk@faculty.iitm.ac.in

ABSTRACT

Co-delivery of two or more drugs either simultaneously or sequentially, commonly referred as the combination therapy being explored to increase the efficacy by targeting multiple interrelated pathways for many treatments. Calcium phosphate (CaP) nanoparticles such as hydroxyapatite (HA), calcium deficient HA (CDHA) etc., have been extensively used as bone substitutes and as drug carriers in various bone and dental applications. Recent advances in CaPs have focused on imparting multi functionality through ionic substitutions for combined applications such as bone regeneration, controlled delivery of drugs and medical imaging. In this talk the potential of CaP nanoparticles as magic bullets with features such as combinatorial drug therapy, extended antibacterial activity and multi-mode contrast ability will be presented. The preparation of ion substituted HA/CDHA through synthetic and natural sources will be outlined. Co-delivery of dual drugs, enhanced regenerative potential and multi-model contrast for CT/MRI imaging of the ion substituted CaP will be discussed. The *in vivo* animal studies on new bone formation of CaP filled cranial bone defects in rat models will also be presented. The scope of multifunctional CaP platforms for the management of bone cancer will be highlighted.

Multi-scale Modeling of Nanomaterials

Prof. Douglas S Galvao

Applied Physics Department, State University of Campinas, Campinas-SP, Brazil

E-mail: galvao@ifi.unicamp.br

ABSTRACT

Carbon atoms exhibit various hybridizations (e.g., 6sp, sp^2, and sp^3), forming a wide array of structures with adjustable mechanical and electronic characteristics. Additionally, these structures can manifest diverse topologies across different electronic dimensions (0 for fullerenes, 1 for nanotubes, 2 for graphene, and 3 for diamond). These topologies have been exploited in developing numerous materials, including bucky papers, carbon nanotube-based artificial muscles, foams, and auxetic crystals. However, the complexity of some of these materials' topologies poses challenges in accurately modeling their mechanical and structural properties. In this presentation, I will introduce and explore multi-scale modeling approaches for these materials, from fully atomistic to macroscale. It will include using artificial intelligence techniques, such as bioinspired ANT algorithms. Particularly noteworthy are the emerging molecular dynamics simulation methods based on reactive potentials, which allow the simulation of multi-million atom systems at a significantly reduced computational cost compared to fully quantum methods. These techniques also extend to non-carbon materials like chalcogenides and the newly realized 2D materials from non-van der Waals solids.

Keywords: Multi-scale modelling; Artificial intelligence; Molecular dynamics simulation; ANT algorithm; multi-million atom.

References:

[1] M. D. Lima et al., Science 338, 6109 (2012).

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Oxides Nanostructures and Engineered Anodes for Rechargeable Zn-ion/Air Batteries

Prof. Ranjit Bauri

Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai, 600 036, India
E-mail: rbauri@iitm.ac.in

ABSTRACT

In the wake of diminishing fossil fuel resources and the ever-increasing demand for energy, a number of energy harvesting, conversion and storage technologies are being actively pursued worldwide. While lithium-ion batteries (LIBs) are the state-of-the-art for powering devices, they suffer from certain limitations such as low energy density, high cost and safety issues. Recently, metal–air and metal-ion batteries have attracted attention as a promising energy storage technology owing to their high theoretical energy density, better safety and abundance. Among these Zn–air and Zn-ion batteries have come to prominence owing to their high theoretical energy density, and favorable electrochemistry of zinc which is also an earth-abundant element unlike lithium. An efficient bifunctional catalyst which can perform both oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) is required for rechargeable Zn-air batteries. Zn-ion batteries on the other hand thrive on the zinc intercalation and stripping capability of the cathode catalyst. Noble metal-based materials such as Pt/C or IrO_2 are well known electrocatalysts but are not cost effective. Transition metal oxides such as MnO_2, Mn-Co oxide exhibit bifunctionality owing to the multiple valence states of Mn and Co. Transition metal vanadium oxides (TMVO) such as zinc vanadium oxide (ZVO) possess a layered structure that enables intercalation of cations while the multiple oxidation state of vanadium maintains electroneutrality. This makes TMVOs suitable cathode catalysts for rechargeable Zn-ion batteries. Co-Mn oxides and ZVO nanostructures were explored in this study as the cathode catalysts for rechargeable Zn-based batteries. Co-Mn oxides with different levels of Mn ($Mn_xCo_{3-x}O_4$) were obtained as nanocages using the zeolitic-imidazolate framework (ZIF) as a template. ZVO nanobelts were processed by a hydrothermal synthesis method. ZIF derived Co-Mn oxide with a Co:Mn ratio = 1 exhibited the best performance signifying the importance of an optimum level of Mn doping. It displayed an onset potential 0.9 V vs RHE and half wave potential of 0.76 V in case of ORR. For OER, the overpotential was observed to be 410 mV to reach a current density of 10 mA/cm^2.These results are comparable to performance of noble electrocatalyst Pt/C. ZVO, on the other hand delivered a specific capacitance of 275 mAh g^{-1} (@ 1 C rate), coulombic efficiency of 99.6 % and 94 % capacity retention after 200 cycles. These results suggest that the studied transition metal oxides are efficient bifunctional cathode catalysts for rechargeable Zn-air/ion batteries. The anode has been engineered in different ways to make it better than commercial Zn (C-Zn) foil anodes. Here we report the engineered anode obtained by electrodeposition of Zn (E-Zn) over Cu foils. The E-Zn anode displayed relatively larger current density and superior rate capability compared to commercial Zn (C-Zn) foil anode. The E-Zn anode also exhibited high capacity retention of ≥97 % after 100 cycles. Thus, this study demonstrates that oxide nanostructures as efficient cathode catalysts and engineered anodes can pave the way for developing high-performance rechargeable Zn-ion/air batteries.

Keywords: Zn-ion battery; Energy storage; Bifunctional catalyst; Nanostructures; Engineered anode.

Operando Microscopy: Correlation of Structural, Chemical and Electrochemical Evolution in Lithium-ion Batteries using Secondary Ion Mass Spectrometry Imaging

S. Eswara*, S. Sharma, and T. Wirtz

Advanced Instrumentation for Nano-Analytics, Luxembourg Institute of Science and Technology, L-4422 Belvaux, Luxembourg

*Corresponding Author E-mail: santhana.eswara@list.lu

ABSTRACT

Advancements in lithium-ion battery technology depend significantly on the availability of sophisticated characterization techniques. However, high-resolution chemical imaging of low atomic number (low-Z) elements such as lithium (Li) presents challenges for conventional chemical analysis methods, including Energy-Dispersive X-ray Spectroscopy. High-resolution Secondary Ion Mass Spectrometry (SIMS) imaging is a well-established technique that facilitates the analysis of all elements, including isotopes. Consequently, SIMS imaging has been extensively employed in Li-ion battery research. While direct imaging of Li in post-mortem battery components provides valuable insights into degradation mechanisms, a comprehensive understanding of Li distribution evolution at high spatial resolution during battery operation ("operando") is critical for studying local interfacial processes, charge transport properties, and degradation pathways. Recent reports have introduced operando Time-of-Flight SIMS imaging for batteries; however, these studies have not achieved the lateral resolution necessary to investigate nanoscale processes [1]. To address this limitation, we developed an innovative operando methodology for Focused Ion Beam (FIB)-SIMS imaging and analysis with sub-20 nm lateral resolution. This methodology utilizes a custom-designed magnetic-sector mass spectrometer [2] integrated with a ThermoFisher SCIOS Ga^+ FIB system for high-resolution SIMS chemical imaging. A specially designed operando sample holder enables electrochemical cycling of batteries within the FIB-SIMS setup. The system leverages the micromanipulator, traditionally used for preparing Transmission Electron Microscopy lamellae, to establish electrical contact with one of the battery electrodes via the operando sample holder, thereby completing the circuit. An external potentiostat drives the charging and discharging cycles of the batteries. Proof-of-concept experiments were conducted using Li|$Li_7La_3Zr_2O_{12}$|Li symmetric half-cells, with galvanostatic cycling performed in situ until sample failure. SIMS chemical mapping revealed lithium redistribution during cycling. Lithium-rich phases emerged, likely percolating through grain boundaries and pores in the solid electrolyte, ultimately causing short-circuit failures. These findings validate our operando methodology, demonstrating its potential to achieve SIMS chemical imaging with sub-20 nm lateral resolution for Li-ion battery analysis [3, 4]. This work was funded by Horizon Europe project OPINCHARGE and by the Luxembourg National Research Fund (FNR) through the grant INTER/MERA/20/13992061 (INTERBATT).

Keywords: Lithium-ion battery; Operando methodology, Li|$Li_7La_3Zr_2O_{12}$|Li symmetric half-cells.

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[4] L. Cressa et al., Electrochimica Acta 494 (2024) 144397

Nano-Materials characterization with Latest Ultra High-Resolution and Analytical Electron Microscopy

T Oikawa [1,*], H. Hashiguchi [2], I. Ohnishi [2]

[1] *JEOL Asia Pte Ltd., #01-12 Corporation Place, 2 Corporation Road 618494, Singapore*

[2] *JEOL Ltd. 1-2 Musashino 3-chome, Akishima, Tokyo 196-8558, Japan*

Corresponding author E-mail: oikawa@jeolasia.com.sg

ABSTRACT

The structural analysis at atomic resolution is requested for characterization of materials, especially for ceramics, functional materials, etc. In order to perform atomic resolution analysis, spherical aberration corrected analytical electron microscopy is becoming widespread, recently (1). In this introductory talk, two types of latest models of advanced analytical electron microscopes are introduced:

One is an aberration corrected 200 kV TEM/STEM, and the other one is a high throughput 200 kV analytical TEM/STEM. Figure 1 shows appearances of microscopes introduced in this lecture; (a) 200 kV FE-TEM, *JEM-F200* and (b) 200 kV aberration corrected, *NEOARM(JEM-ARM20F)*. The cold or Schottky FEGs are selectable in the F200, and the cold-FEG is configured in the NEOARM as a standard. The high efficiency dual type X-Ray detectors are installed in both. Advanced higher-order aberration correctors (2) are installed in the *NEOARM*. The accelerating voltages are variable from 20 to 200 kV in *F200* and from 30 to 200 kV in *NEOARM*. All the analytical instruments, such as STEM detectors, EDS(SDD), EELS are fitted inside of cover panels designed for anti-acoustic, anti-magnetic and thermal protective. Owing to higher coherent electron of cold-FEG and advanced aberration-corrector combination, TEM lattice resolution of 70 pm is obtained in NEOARM. And owing to small source size of cold-FEG and advanced aberration-corrector combination, STEM resolution of 71 pm is obtained in NEOARM(UHR).

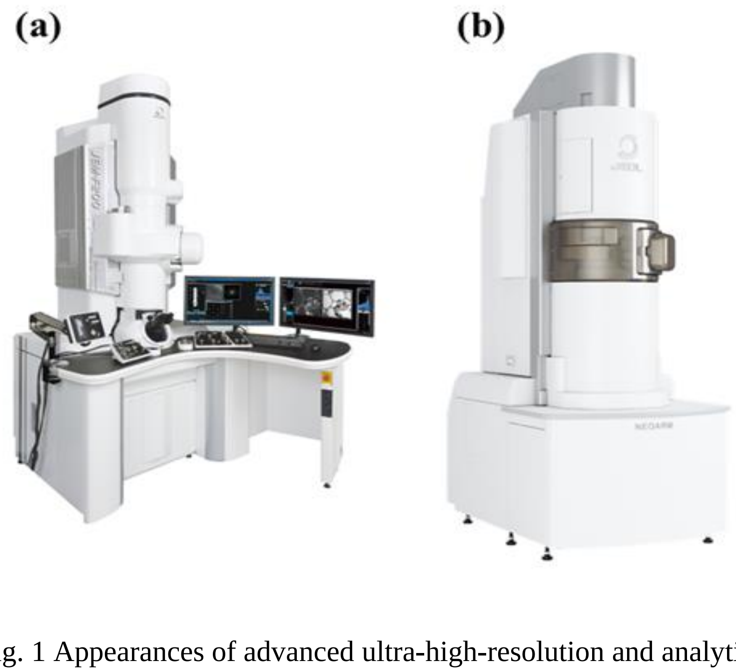

Fig. 1 Appearances of advanced ultra-high-resolution and analytical electron microscopes.
(a) *JEM-F200* 200 kV High Throughput Analytical TEM/STEM.
(b) *NEOARM* (*JEM-ARM200F*) 200 kV Aberration Corrected Analytical TEM/STEM.

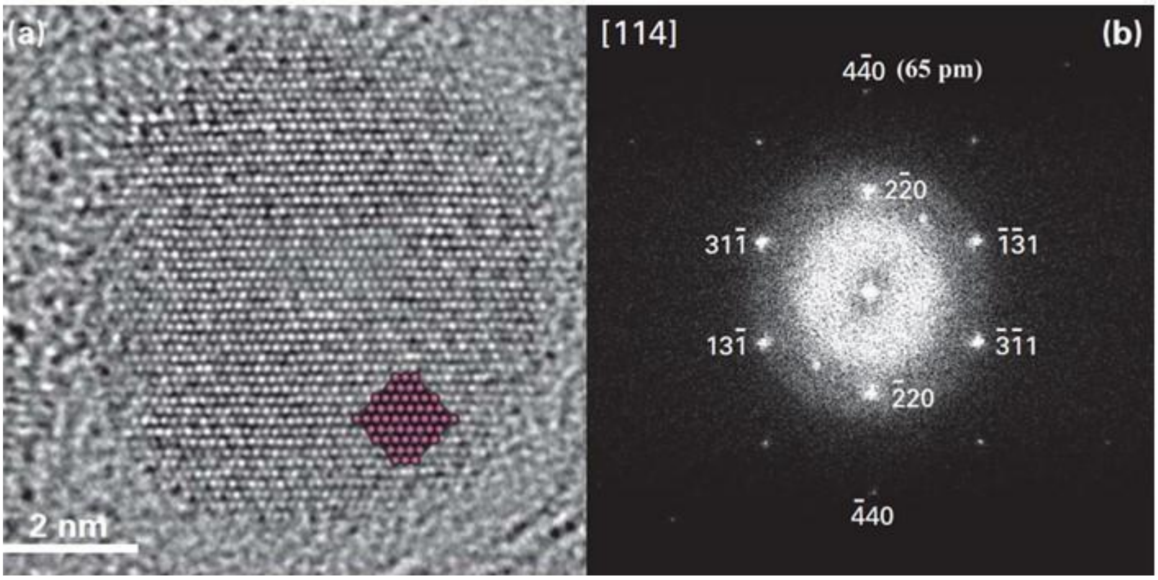

Fig. 2(a) Aberration corrected HRTEM image of a CoPt nano particle observed along the [114] zone-axis orientation (Cs = 0.005 mm), Df = - 0.5 nm (Scherzer focus), focus spread of 2.2 nm). An inset (red illustration) indicates an atomic model on the projected crystal plane. (b) Corresponding diffractogram (power spectrum) of the HRTEM image (a). It is showing of the 65 pm resolution for atomic spacing at (440) lattice spacing.Figure 2 shows an example of ultra High-Resolution (HRTEM) image (Fig. 2 (a)) of a CoPt nano particle in the [114] zone axis orientation which is directly observed on the Cs-corrected HR image and an information transfer up to the (440) reflection (65 pm) is reported on the diffractogram (Fig. 2(b)).It is investigated that highlight the performance of aberration-corrected HRTEM to extract quantitative information from dynamical process with single atom sensitivity, which can provide better insights into the characterization of crystal growth or catalytic reactions.

In the lecture, practical application data analyzed with both *F200* and *NEOARM*, is introduced.

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Covalent Organic Framework Membranes for Molecular Separations and beyond

Dr. Bishnu P. Biswal

School of Chemical Sciences, National Institute of Science Education and Research (NISER) Bhubaneswar, Jatni, Khurda, Odisha 752050, India

E-mail: bp.biswal@niser.ac.in

ABSTRACT

Membrane-based separation is vital in various industrial processes because of its low energy consumption, compact design, and ease of operation. The advancement of this technology hinges on the development of innovative membrane materials. While polymer-based membranes have been used for a long time, their efficiency is limited by the trade-off between permeability and selectivity. Thus, the quest for novel membrane materials is a primary focus for academia and industry. Nanoporous materials such as zeolites, metal-organic frameworks (MOFs), and covalent organic frameworks (COFs), based membranes provide better separation performance due to their ordered porous structures. COFs, in particular, are promising for advanced gas and liquid-phase separation processes because of their crystalline nature, well-defined porosity, tunable functionalities, and versatile architectures. Since the first COF membrane (COFMs) for gas separation was introduced in 2015, there has been rapid progress in their development, underscoring their potential in membrane-based separations of gas mixtures (CO_2/N_2; CO_2/CH_4; H_2/N_2 etc.), molecular separation (ions and dye separation), solvent nanofiltration, oil-water separation and more. Not limited to molecular separation, recently, COFMs have also emerged as potential semiconducting materials for photonics and optoelectronic device applications. The optical conductivity of free-standing 3D COFMs using TeraHertz (THz) spectroscopy and nonlinear optical (NLO) response of free-standing COFMs along with molecular separation potentials of inhouse developed COFMs were studied.

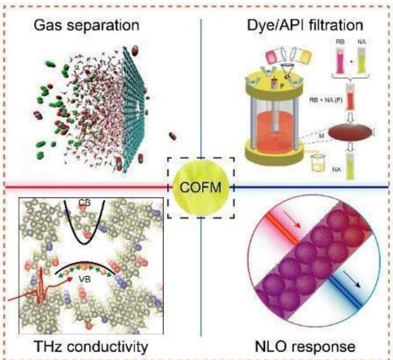

Figure 1. *Schematic of the distinct applications of COFMs for molecular separation and light-matter interaction.*

Keywords: Membrane-based separation; Metal-organic frameworks; Covalent organic frameworks; TeraHertz spectroscopy; Nonlinear optical response.

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Synthesis of Self-Assembled Nanostructured Liquid Cisplatin via Supercritical CO_2 Processing

Prof. Sudhir Kumar Sharma

Engineering Division, New York University Abu Dhabi, Abu Dhabi, UAE

E-mail: sks16@nyu.edu

ABSTRACT

Cisplatin is one of the most potent chemotherapeutic drugs used for the treatment of numerous solid tumor malignancies. Clinical treatment with cisplatin causes severe side effects such as kidney damage, allergic effect, hearing loss, etc. While it is very effective against some cancers, severe toxicity and poor aqueous solubility limits widespread use in drug delivery. To formulate a better tolerated and more water-soluble form of cisplatin, we report a custom designed RESS process for the synthesis of a novel, amber-colored and viscous aqueous cisplatin solution (denoted as *liquid cisplatin*) with increased solubility and storage stability. Extensive material characterizations of these solutions were carried out to determine any chemical and/or structural changes of the *liquid cisplatin*. Using specialized liquid cell in situ transmission electron microscopy (liquid in-situ TEM) and Raman spectroscopy, we demonstrated that *liquid cisplatin* comprises a bi-modal distribution of a highly solvated network of stable cisplatin nanoclusters in water and exhibited 27× greater water solubility than standard cisplatin. More importantly, *liquid cisplatin* was stable at ambient conditions for over two years. Extensive analytical characterization of *liquid cisplatin* confirmed that it retained the original chemical identity of cisplatin. Cell viability and apoptosis studies on human lung adenocarcinoma A549 cells provided compelling evidence that *liquid cisplatin* demonstrated a more sustained anticancer effect compared to standard cisplatin. In vivo studies revealed that standard cisplatin solutions were acutely toxic and caused death of rapidly proliferating cells compared to our cisplatin, which were better tolerated with reduced general cell death. Increased water solubility (i.e., up to 27 times) and matched chemical identity of *liquid cisplatin* indicate the possibility of developing non-invasive and highly effective novel cisplatin drug-delivery platforms.

Keywords: Cisplatin; RESS process; Poor aqueous solubility; Liquid cisplatin.

Room Temperature Hydride ion Conduction in Rare-Earth Oxyhydroxides

Dr. Soshi Iimura

National Institute for Materials Science, Japan

Corresponding Author E-mail: llMURA.Soshi@nims.go.jp

ABSTRACT

Hydride ion (H^-) is a unique anionic species that exhibit high reactivity and chemical energy. H^- conductors are key materials to utilize advantages of H^- for applications, such as chemical reactors and energy storage systems. However, low H^- conductivity at room temperature (RT) in current H^- conductors limits the applications. Recently, H^- conductivity of ~1 mS cm^{-1} at RT is observed in $LaH_{3-2x}O_x$ with x < 0.25, which is higher by 3 orders of magnitude than that of the best H^- conductor [1, 2]. The oxygen concentration (x) is crucial in achieving fast H^- conduction near RT; the low activation barrier of 0.3–0.4 eV is attained for x < 0.25, above which it increases to 1.2–1.3 eV. Molecular dynamics simulations using neural-network potential successfully reproduced the observed activation energy, revealing the presence of mobile and immobile H^-. In this talk, in addition to the ionic conduction properties, the thin film device using the H^- conducting rare-earth oxyhydrides [3] is also presented.

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ICME and Microstructure Informatics framework for the Alloy Design

Dr. Rahul M R

Department of Fuel, Minerals and Metallurgical Engineering, Indian Institute of Technology (ISM) Dhanbad, Jharkhand, 826004, India

E-mail: rahulmr@iitism.ac.in

ABSTRACT

The design of multicomponent alloys is challenging due to the large compositional space and requires a series of experiments and resources. Integrated Computational Materials Engineering (ICME) has shown promising results for new material development with less experimentation and time. Simulation-guided experiments reduced the usage of resources. Recently, the application of machine learning and deep learning in alloy design and development has shown remarkable improvement in new material prediction. A material informatics workstation is proposed for industrial applications. The talk will focus on developing the ICME + ML framework to design and develop new high-entropy alloys in the solidification route. Applying computer vision and deep learning will assist in various length scales of material structure identifications. These have the potential to predict the microstructure in various conditions. The talk also discusses a few studies from microstructure informatics and proposes an ICME + microstructure informatics framework for alloy design and development.

Keywords: Materials informatics; ICME; Microstructure Informatics; High Entropy Alloys.

Correlative Microscopy and Controlled Electron Channeling Contrast Imaging – A New Perspective for Defect Analysis in Bulk Samples

Satya Srinivas B

Carl Zeiss India Private Limited, Bangalore, India

Corresponding Author E-mail: satya.srinivas@zeiss.com

ABSTRACT

The pursuit of innovation in characterization of materials- particularly in energy, environment and health care materials research necessitates comprehensive multi-scale investigations and the ability to correlate diverse experimental data at the same region of interest. Understanding the intricate behavior of these materials across varying length scales in multi dimensions is critical to uncovering the structural parameters that dictate performance, efficiency, and endurance. The major development enabling correlation is the recent development of a modern microscopy workflow environment (ZEISS Atlas 5), which acts as the interface between experiments obtained on multiple platforms (SEM, LM, FIB-SEM, XRM, etc.). By combining advanced imaging, analytical, and correlative techniques, Zeiss offers a seamless approach to bridging nanoscale insights with macroscale understanding, empowering researchers to decode the complexities of energy materials. This talk will also highlight about new approach to characterize dislocations in bulk samples with a scanning electron microscope (SEM) which is controlled Electron Channeling Contrast Imaging (cECCI). This cECCI technique will explore how to visualize crystallographic defects in polycrystalline materials using controlled electron channeling contrast imaging (cECCI) in an SEM.

Keywords: Material characterization; Advanced imaging techniques; Multi-scale investigations.

Piezoelectric materials for energy harvesting and pressure sensing applications

Subash Cherumannil Karumuthil

Center for Nano and Soft Matter Sciences, Bengaluru, 562162, India

Corresponding Author E-mail: cksubash2020@gmail.com

ABSTRACT

The potential of piezoelectric materials to transform mechanical strain into electrical energy has attracted a lot of interest in the realm of flexible electronics. The piezoelectric nanogenerator is a crucial part of renewable energy in a time when conventional energy sources are running limited.Piezoelectric nanogenerators (PENG) can be used in a variety of applications, such as pressure sensors, biological sensors, tactile sensors, and wearable energy harvesting systems. Numerous attempts have been made to enhance the well-known polyvinylidene fluoride's piezoelectric capability. Current research endeavors concentrate on augmenting PVDF's piezoelectric properties by the integration of nanomaterials[1,2]. Although the basic principles of nanomaterial selection are yet unknown, this field of study examines a variety of nanomaterials. In this talk I would like to cover some of our recent findings on the direction of mechanistic aspects of polymer and nanomaterials interactions which leads to the enhancement of piezoelectric property of the PVDF. Specifically transition metal dichalcogenides (TMDs), the 2D materials can be utilized as a nanoadditive for enhancing the characteristics of piezoelectric polymer. Vanadium-disulfide (VS_2), one of the TMD, is introduced into this field to improve the energy generation properties of the polymer[1]. The high surface charge and minimal addition of VS_2 nanomaterial can able to achieve better piezoelectric performance. The optimized combination was well studied and a working prototype of energy harvesting and pressure sensing device was fabricated by proper packaging by considering the long term usage. The real time demonstration as a road safety and smart door sensor prove that the new polymer nanocomposite will be a potential candidate for developing highly efficient, flexible and sensitive energy harvesting and pressure sensing devices. Metal organic frame work derived Zirconia nanoparticles were used to study the effect of crystal structure and surface characteristics of the filler on electroactive phase of the polymer[2]. To study the influence of the crystallographic phase on the electroactive phase of PVDF polymer, The polymer nanocomposite with monoclinic zirconium oxide filler derived from UiO-66 has shown better enhancement in β phase when compared with other nanofillers that were studied. It is hypothesized that the more hydrophobic monoclinic phase (ZrO_2-66m) may be acting as a better nucleating agent leading to a better interaction with PVDF. Piezoelectric devices were fabricated with polymer nanocomposite films and tested, the output results are in line with the material characteristics. A real time practical demonstration of prototype was carried out by installing the prototype in a pavement and used it for different applications. The pavement prototype was used to power LEDs and charge a 1 µF capacitor to demonstrate the energy-generating and storing performance. The pavement prototype was also demonstrated at a laboratory scale as a wireless security alert system.

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Company Malvern Panalytical, a division of Spectris Pvt Ltd
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ABSTRACTS FOR ORAL/POSTER

AB 102

Effect of Zircon flour and MoS2 Powder on Coefficient of Thermal expansion of ZA-27 Composites

Gurunagendra G R[1,*], Shreekala N[2], Raju B R[3], **V Ravikumar[4]**, Anil Kumar K S[5]
Siddesha H S[6]

[1,2,4]*Department of Mechanical Engineering, Global Academy of Technology, VTU Bangalore, 560098, India*

[3]*Department of Mechanical Engineering, The Oxford college of Engineering, Bangalore 560068, India*

[5]*Department of Mechanical Engineering, JSS academy of Technology, VTU Bangalore, 560060, India*

[6] *Department of Mechanical Engineering, ACS college of Engineering, Bangalore 560074, India*

*Corresponding Author Email: gurunagendra.gn@gmail.com

ABSTRACT

Stir casting was used to prepare ZA-27 composites with weight fractions of 1.5 wt.%, 3.0 wt.%, 4.5 wt.%, and 6.0 wt.% of ceramic zircon flour ($ZrSiO_4$) particles and 3wt. % Molybdenum di sulphide (MoS_2) lubricant particles. We discovered the morphological structure, density, and void fraction of ZA-27/$ZrSiO_4$/MoS_2 composites. The effect of zircon flour particles and MoS_2 as reinforcement, as well as the fabrication technique, are being investigated. Use of MoS_2 as dry lubricant minimizes the use of external lubricant for reducing friction there by reducing cost and improving sustainability. After casting the composite samples in the shape of rods they were designated as per weight fraction and evaluated for density and porosity. SEM/EDAX was used to determine the distribution of reinforcement particles and chemical composition in ZA-27 composites. Coefficient of thermal expansion (CTE) of the ZA-27 composites and ZA-27 hybrid composites are evaluated using a standard dilatometer device followed by Finite element simulation and Rule of mixture to study the effect of reinforcement on CTE.

Keywords: SEM; EDAX; Porosity; MoS_2; Dilatometer.

AB 103

Mxene- Layered Double Hydroxide Layers Coated AZ31for Corrosion Resistance Applications

Juvairia K K[1] and P Amaravathy [2,*]

[1]*Dr. NGP Arts and science college, Coimbatore, Tamilnadu, India- 641035*

[2]*PPG Institute of Technology, Coimbatore, Tamilnadu, India- 641035*

[*]Corresponding author E-mail: amaravathybme.it@ppg.edu.in

ABSTRACT

Metallic alloys serve as fundamental materials in a diverse array of engineering applications, cherished for their remarkable mechanical properties and resistance to corrosion. Magnesium and its alloys are characterized by low density (1.74–1.95 g/cm^3), high strength-to-weight ratio, non-toxicity, biocompatibility, and good machinability. Magnesium (Mg) alloys are frequently employed in automotive and aircraft applications owing to their remarkable strength-to-weight ratios. Particularly, magnesium-aluminium (Mg-Al) alloy systems exhibit outstanding mechanical performance, ease of processing, and cost-effectiveness. However, the susceptibility of AZ31 alloy to corrosion in specific environmental conditions acts as a significant impediment, formation of a more homogeneous microstructure with a low dislocation density curtailing its widespread practical applications. In order to slow down the degradation various surface modification studies and coatings have been attempted on magnesium alloys for various applications. The present study deals with the improved corrosion resistance of functionalised Ti_2N MXene- Layered Double Hydroxide layers coated AZ31 by hydrothermal method. The electronegative mainboard of MXene possess fluoride ion and this adsorb the cations on the surface, leading to the growth of Layered Double Hydroxides (LDH). The coating is dense, complete and intrinsic tunnels made by LDH sheets make it more resistant to corrosion. The composition of the coating is characterised by its respective XRD peaks. The corrosion test was carried out by immersing the samples in 3.5 wt % NaCl solution and the results showed that the functionalised MXene/MgAl-LDH-coated AZ31 alloy showed improved corrosion resistance and this can prevent the corrosive species from reaching the substrate effectively. The i_{corr} values of coated alloys are very low for functionalised MXene/MgAl-LDH coated alloy compared to bare alloy as evidenced from potentiodynamic polarisation studies. Hence, this simple and facile work helps to improve the corrosion resistance of magnesium alloys and opens a new perspective for anticorrosion application with the emerging 2-Dimensional MXene materials.

Keywords: MXene; Magnesium; Potentiodynamic polarisation; Hydrothermal; Corrosion; Titanium nitride.

AB 110

Development and Characterization of Cocos Nucifera Shell (CNS) Biochar Reinforced Vinyl Ester Composites

M Aravindkumar[1,*], K Ashwin[1], B Balavairavan[2], B K Parrthipan[2], S Thanga Kasirajan[3]

[1] *UG, Second Year Students, Department of Mechanical Engineering, Kamaraj College of Engineering and Technology, Virudhunagar*

[2] *Assistant Professor, Department of Mechanical Engineering, Kamaraj College of Engineering and Technology, Virudhunagar*

[3]*Associate Professor, Department of Mechanical Engineering, Kamaraj College of Engineering and Technology, Virudhunagar**Corresponding Author E-mail: m.aravindkumar765@gmail.com

ABSTRACT

Biochar derived from farm waste such as coconut (***cocos nucifera***) shell was utilized to derive the biochar by pyrolysis process at 600°C. The surface properties of CNS biochar was enhanced by 5% of NaOH treatment. The different proportions (5, 10 15wt. %) of untreated and alkali-treated ***cocos nucifera* shell (**CNS) biochar reinforced with vinyl ester resin (VER) to fabricate the composite plates by solution casting method. The ultimate purpose of this work is to maximize the utilization of agricultural wastes and their carbonaceous bio-fillers to enhance the mechanical, thermal, viscoelastic, physio-chemical, and electrical properties of polymeric composites. Alkali treatment of the *Cocos nucifera* shell (CNS) biochar results in the removal of non-cellulosic components and the elimination of dust particles. According to experimental findings, the properties of the VER/a-t CNS biochar composites were superior to VER/CNS biochar composites. The FTIR analysis showed that, due to alkali treatment the chemical functional groups of matrix and fillers are almost the same and there is no formation of new chemicals. The crystallinity index and crystalline size of the composite with treated biochar are higher than untreated biochar samples. The maximum degradation temperatures for untreated and alkali-treated CNS biochar were 465°C and 475°C, respectively, while the pure vinyl ester plate exhibited a degradation temperature of 353°C. The DSC results showed that the crystallization temperatures of the pure vinyl ester plate, VER/15 wt. % CNS, and VER/15 wt.% a-t CNS composites are 102.04°C, 118.65°C, and 124.54°C, respectively. The thermal conductivity of the composite reached up to 2350 J/kg.K, confirming that the alkali-treated CNS biochar acted as a rigid filler and enhanced the thermal stability of the composites. The incorporation of CNS biochar improved the tensile, flexural, storage modulus, and impact strength of vinyl ester plates. The best mechanical properties were achieved with 15 wt. % alkali-treated CNS biochar due to better surface strength, stress transfer, and dispersion. The composites exhibited the flexural strength of 39.1 MPa and 52.5 MPa and a flexural modulus of 1.46 GPa and 1.73 GPa for 15 wt. % of untreated and alkali-treated CNS biochar, in vinyl ester matrix respectively. The tensile strength of 42.9 MPa and tensile modulus of 1.34 GPa were absorbed for VER/ 15 wt. % a-t CNS biochar composites. The VER/15wt. % a-t CNS composites withstand the impact energy of 12.9 kJ-m^2. The VER/CNS biochar composites only conducted electricity with 15 wt. % of alkali-treated and untreated CNS biochar, showing electrical conductivity of 0.019 S/m and 0.034 S/m, respectively. Based on the outcomes of various characterization techniques, the alkali-treated *Cocos nucifera* shell (CNS) biochar acts as a rigid filler in the vinyl ester matrix, creating composites with excellent mechanical, thermal, viscoelastic, and electrical properties. It also helps maximize the use of biochar from farm waste for various industrial applications.

Keywords: ***Cocos nucifera*** shell (CNS); Alkali-treated biochar; Farm industrial waste; Electrical conductivity; Tensile strength.

AB 111

Morphology Tuning and Interfacial Tension-Impelled Self-Assembly of Poly(3,4-ethylene dioxythiophene)/Tellurium Nanocomposites at Various Liquid/Liquid Interfaces

Nesleena Puthiyottil[1], Subramanyan Namboodiri Varanakkottu, and Mini Mol Menamparambath[2*]

Department of Chemistry, National Institute of Technology Calicut, Calicut, Kerala 673601, India

*Corresponding Author E-mail: minimol@nitc.ac.in

ABSTRACT

Compared to the enormous number of nanostructures that have been documented, the variety of nanostructures produced by organic polymerization is rather limited. We devised an unconventional route and a sustainable approach to distribute tellurium nanoparticles (TeNPs) in poly(3,4-ethylene dioxythiophene) (PEDOT) matrix to form a semiconducting organic-inorganic nanocomposites for potential applications in electrochemical sensing. The adopted strategy of in situ liquid/liquid interface-assisted polymerization aids the formation of intimately and permanently tethered TeNPs on the PEDOT polymer chains, thereby preventing the aggregation of TeNPs. The untapped versatility is inherent to using biphasic systems for interfacial polymerization explored at three interface systems of immiscible solvents: chloroform/water (C/W), dichloromethane/water (D/W), and hexane/water (H/W) giving rise to PEDOT/Te nanocomposites (PTeNC) of distinct morphology. XRD and Raman analysis proved the successful formation of PTeNC in all the systems. The choice of solvents and the resultant IFT played a significant role in tuning the morphology of PTeNC. Consequently, when the product confinement took place at the interface and the bulk phase, respectively, 2D nanosheets as well as core−shell structures were formed. This diversity in morphology was confirmed from HR-SEM, HR-TEM, and AFM images. When PTeNC was synthesized in C/W, ultrathin sheets were produced, followed by small sheets and nanospheres in D/W, and then clearly distinguishable core−shell structures in H/W. PTeNC in all the solvent environments was eventually compared for their electrochemical activity for the enzyme-free detection of ascorbic acid (AA). In contrast to other composites, PTeNC (H/W) had a distinct irreversible oxidation peak for AA. A 3 wt % MWCNT integration into PTeNC (H/W) elevated the current response 2-fold with a LOD of 0.66 μM and excellent sensitivity, anti-interference ability, and reproducibility. Taken together, we envision that the L/L interface-aided strategy of polymerization can be immediately extended to construct diversified and complex structures and compositions when the precursors are appropriately chosen for promising applications in thermoelectrics, optics, optoelectronics, sensors, energy conversion, storage, etc. Also, we envisage that the current work not only offers a facile approach to synthesizing and tuning the morphology of a fascinating array of intimately contacted organic−inorganic nanocomposites at various L/L interfaces but also opens a new alleyway of utilizing unusual metals as electrode materials to widen the scope of biosensors.

Keywords: PEDOT/Te nanocomposites; Liquid/liquid interfaces; Interfacial tension; Ascorbic acid; Non-enzymatic electrochemical sensor.

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Investigation of Ternary Blends with Nanomaterial on CI Engine for Environmental Protection

Ganesh Chembedu*, P V Manu, Naveen K
Department of Mechanical Engineering, NIT Calicut, Kozhikode, India
*Corresponding author Email: chembeduganesh@gmail.com

ABSTRACT

The researchers demonstrated that biodiesel is a viable substitute for standard diesel fuel. It does, however, increase emissions of nitric oxide. The current study examines the performance and emissions of the blend of the nano additive material titanium dioxide-TiO_2 with watermelon seed oil biodiesel (WSB) and isopentanol (IP) by adopting preheating and EGR in a diesel engine. WSB and IP are taken at varying concentrations (5%, 10%, 15%). For effective and clean combustion, concentrations of 30, 65, and 100 ppm of the non-toxic, non-corrosive, chemically stable, and thermally stable nanoparticles (NPs) TiO_2 is used. The test results are analyzed using the Technique for Order Preference by Similarity to Ideal Solution (TOPSIS) approach. As indicated by the analysis of experimental results, WSB15IP15NP30 is the ideal TOPSIS fuel blend with nanomaterial. The WSB15IP15NP30 blend, when compared to diesel, increases BTE by 4.7% and decreases NO_x, smoke, HC, BSEC, CO, and CO_2 by 47.7%, 21.2%, 16.4, 16.4%, 12.7%, 9.1%, and 1.4% respectively. Titanium dioxide nanomaterial has reduced emissions, which makes it a material for environmental protection. Overall, it is determined that nanomaterial TiO_2-30 ppm coupled with (WSB15-IP15-diesel) fuel is a superior substitute to diesel for unmodified CI engines.

Keywords: Biodiesel; Alcohol; Optimization; Emissions; Performance.

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Non-Surgical Non-Adhesive Smart Hearing Aid Using Bone Conduction Transducers

A M Shah[1,*], Vasif Ahmed[2]

[1]*Electronics and Telecommunication Engineering Department, Government College of Engineering Amravati, Amravati M.S. India;*
[2]*Electronics and Electrical Engineering Department, Babasaheb Naik College of Engineering, Pusad M.S. India*
*Corresponding Author E-mail: shah.ameed@gcoea.ac.in

ABSTRACT

The non-surgical non-adhesive smart hearing aid glasses are developed for the deaf people suffering from conductive hearing loss. Piezoelectric transducers are used as the bone conduction transducers making these hearing aid glasses the most power efficient, lightweight, compact and reliable hearing aid. The non-surgical and non-adhesive feature is achieved by using the glasses as the body of hearing aid. This makes the hearing aid glasses the most safe and affordable bone conduction aid in comparison to the surgical impact or adhesive bone conduction aid. A novel technology used in these hearing aid glasses is a new type of flexible piezoelectric based bone conduction transducer. The used piezoelectric transducers are unidirectional i.e. producing vibration only from one side (further the other side should have a layer of material absorbing vibrations, thereby increasing its directivity). For our application the newly developed transducer should have the ability to produce sound vibrations of different frequency ranges from the same surface. It is very power efficient as it consumes power in milliwatts. This drastically improves the battery life of hearing aids.

Keywords: Non-surgical; Non-adhesive; Conductive hearing loss; Piezoelectric transducers.

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Effect of Corona Treatment on Physico–Chemical, Mechanical, Water Barrier, UV-Barrier, and Biodegradation Properties of PVA/Vigna Mungo Husk Powder Reinforced Biofilms

D V Sahi, M Varuneeshbala, B Mayil kani, S Yokahariharan, B Balavairavan, B K Parrthipan,

S Thanga kasirajan

Department of Mechanical Engineering, Kamaraj College of Engineering and Technology, Virudhunagar

*Corresponding Author E-mail: rajini.vignes@gmail.com

ABSTRACT

To substitute the synthetic non-biodegradable plastics in packaging applications, the polyvinyl alcohol (PVA) /Vigna Mungo Husk Powder (VMHP), the biodegradable films were prepared by solution casting method with varying concentrations of VMHP (5–20 wt%) in PVA matrix. This study investigates the effect of corona treatment on the characterization properties of polyvinyl alcohol (PVA)/Vigna mungo husk powder-reinforced biocomposite films. The aim is to enhance the surface energy of PVA/VMHP films by using high-frequency corona discharge and to improve the mechanical properties, water barrier, UV- barrier, and ink adhesions. The treated and untreated biocomposite films were characterized by physiochemical analysis, tensile testing, scanning electron microscopy (SEM), thermal gravimetric analysis (TGA), UV-barrier properties, water absorption test, and soil burial test to evaluate the physical structure, mechanical strength, thermal stability, moisture resistance, optical properties, water absorption, and biodegradation properties. Based on the results obtained, the FTIR spectrum of these PVA/VMHP biofilms suggested that strong hydrogen bonding takes place due to interfacial exchanges of VMHP in the PVA matrix. The XRD results showed that the crystallinity of PVA/VMHP biofilms is greater than the PVA matrix. Thermogravimetric analyses revealed that the thermal stability of PVA/VMHP biofilms improved by 25% due to corona treatment. The light is 45% for transmittance in the visible light region for the PVA/VMHP (20 wt.%) biofilm. The FESEM micrographs of biofilms showed the formation of good physical interaction and compatibility between the polymer matrix and VMHP after corona treatment. The PVA/VMHP corona-treated biofilms with 20% VMHP gave the highest tensile strength and Young's modulus 32.5 MPa and 41.3 MPa, respectively. Additionally, the water absorption rate was reduced, suggesting improved barrier properties. The solubility, water absorption, and WVT of the PVA/VMHP biofilms improved after the corona treatment. These findings indicate that corona treatment is an effective method for optimizing the performance of PVA/Vigna mungo biocomposite films, making them suitable for sustainable packaging and other applications.

Keywords: Vigna mungo husk powder; Corona treatment; Water Solubility; UV-barrier films.

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Soil Mimetic Eco-Friendly Fertilizer Gate: Nanoclay Reinforced Binary Carbohydrate for Crop Efficiency

Parul Sharma[1], Bandana Kumari sahu[2], Vijayakumar Shanmugam[*]

Chemical Biology Unit, Institute of Nanoscience and Technology, Knowledge City, Sector-81, Manauli, S.A.S. Nagar, Mohali -140306, Punjab, India

*Corresponding Author E-mail: psvijayakumar@inst.ac.in

ABSTRACT

Potassium plays a crucial role in crop physiology, hence recommended as a basal macronutrient. But its high mobility, and quick leaching makes it phyto-unavailable, hence nano material-assisted coating on muriate of potash is attempted for the first time, which serves 80% of potassium fertilizer requirement. Rotary drum coating method has been used to coat binary carbohydrate viz., chitosan and lignin with anionic clay as a reinforcing agent that favors the formation of stable coordination bonds. Thus, coated fertilizer fulfills industrial demands like resistance to abrasion and storage. Finally, the coated fertilizer was able to improve the wheat production efficiency to ~ 17 %. While in the function, clay stake to extend the diffusion time and recalcitrant lignin gives cation exchange capacity assisted nutrient feeding as well as laccase induced slow release function. The coating matrix has improved the stability of lignin against laccase significantly to complement the slow release and efficiency.

Keywords: Potassium; Chitosan; Lignin; Nanoclay; Wheat.

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Accelerating Discovery of Non-Equimolar Refractory High-Entropy Alloys Using Machine Learning and Edge Dislocation Theory: A Case Study on the MoNbTiVZr System

Ajimshad A and Anand Sekhar R*

Department of Mechanical Engineering, TKM College of Engineering, Kollam, Kerala, India

*Corresponding Author E-mail: ajimshad@tkmce.ac.in

ABSTRACT

This study expands the exploration to non-equimolar RHEAs by integrating machine learning (ML) techniques and edge dislocation theory to predict new alloy phases and mechanical properties. A methodology was developed that combines ML with phase prediction for non-equimolar compositions, specifically focusing on the MoNbTiVZr quinary alloy system due to its established contributions to high-temperature structural applications. The ML model was trained on a dataset of 1408 high entropy alloys using five algorithms: K-Nearest Neighbors (KNN), Support Vector Machines (SVM), Decision Tree (DT), Random Forest (RF), and Gradient Boosting (GB). Bayesian Optimization (BO) was employed to fine-tune the models, with the Random Forest model achieving an accuracy of 93.5% for predicting single BCC solid solution (SS_BCC) phases. This method was applied to explore the compositional space of the MoNbTiVZr system, with atomic percentages incremented by 5%. The $Nb_{0.6}Mo_{0.05}V_{0.2}Ti_{0.05}Zr_{0.1}$ composition was identified as having a high specific yield strength, predicted using edge dislocation theory. The proposed alloy undergoes mechanical alloying for experimental validation, followed by microstructural analysis using X-ray diffraction (XRD) and scanning electron microscopy (SEM). This approach demonstrates the potential of ML and theoretical modelling to accelerate the discovery of novel, high-performance RHEAs for advanced applications.

Keywords: Refractory High Entropy alloy; Machine Learning; BCC Solid Solution.

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Electrodeposited TiNi Cathodes for Magnesium Based Primary Seawater Batteries

Ayisha Hamdath K K [1] **,** Fathima Fasmin[2,*]

Department of Chemical Engineering, National Institute of Technology Calicut, Kozhikode, Kerala, India

*Corresponding Author E-mail: fathimafasmin@nitc.ac.in

ABSTRACT

Seawater batteries (SWBs) operate on readily available and plentiful electrolyte—seawater; and so, they are a promising sustainable energy source for underwater and maritime applications. In a primary magnesium seawater battery (MgSWB), Mg oxidation occurs at the anode and Oxygen Reduction Reaction (ORR) or Hydrogen Evolution Reaction (HER) occurs at the cathode. One of the major challenges of MgSWB is the lack of cost effective and high performing cathode material, which can replace platinum. In this study, we developed a Ni catalyst electrodeposited on Ti foil (TiNi), that can be used as an efficient cathodic material in MgSWB. The synthesized TiNi cathode was characterized in a three-electrode experimental set up using electrochemical techniques such as cyclic voltammetry, linear sweep voltammetry and electrochemical impedance spectroscopy. Furthermore, the galvanostatic discharge tests using Mg alloy (AZ61) as the anode and TiNi as cathode were conducted. The electrochemical performance of TiNi cathode was compared with that of the benchmark catalyst- platinized carbon cloth (PtC). It was observed that TiNi electrode demonstrated consistent discharge performance that was comparable to that of commercial PtC electrode. At a current density 10 mA/cm^2, the average cell potentials of the AZ61-TiNi and AZ61-PtC cells were 1.42 V and 1.85, respectively.

Keywords: Seawater Batteries; Magnesium Seawater Batteries; Electrodeposition; Cathode; Oxygen Reduction Reaction.

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Machine Learning-Guided Design and Characterisation of CSP-Reinforced High Entropy Alloy Composites

Renju C Daniel[1,2], Mohammed Mudassir[3] , C N Shyam Kumar[3], Anand Sekhar R[1,2*]

[1]*Department of Mechanical Engineering, TKMCE, Kollam 691005, Kerala, India*

[2]*APJ Abdul Kalam Technological University, CET Campus, Thiruvananthapuram,695016, Kerala, India*

[3]*Department of Materials Science and Engineering, NIT, Calicut, 673601, Kerala, India*

*Corresponding Author E-mail: anand@tkmce.ac.in

ABSTRACT

This study presents a novel approach to enhancing High Entropy Alloy (HEA) composites reinforced with Coconut Shell Pyrolyzed (CSP) particles by integrating machine learning techniques and innovative material design. A comprehensive methodology is employed to detect HEA phase composition, combining advanced machine learning algorithms such as Support Vector Machine(SVM), Random Forest (RF) and extreme Gradient Boost (XGBoost) algorithms with experimental validation. Comparative analysis reveals that Valence Electron Concentration (VEC) and mixing enthalpy (ΔHmix) as the most influential parameters. Random Forest algorithm showing superior performance, achieving a test accuracy of 0.7838 and the highest precision score of 0.8767, while maintaining stable cross-validation results. The research methodology involves the fabrication of AlCoCrFeNi-HEA and HEA based composites reinforced with 1 wt% and 2 wt% CSP particles using powder metallurgy and Spark Plasma Sintering (SPS) techniques. The composites are subsequently characterized through X-ray Diffraction (XRD) and Scanning Electron Microscopy-Energy Dispersive Spectroscopy (SEM-EDS) analyses. The reliability of the machine learning model is validated through experimental characterization. XRD analysis reveals a dual-phase (FCC + BCC) structure in the sintered composites, which aligns consistently with the predicted phase structures from the RF model. The validation of the RF model's reliability establishes it as a robust tool for HEA phase prediction, providing a framework to accelerate the discovery and optimization of novel high-entropy alloy compositions and their composites. The results of this research advance the continuous evolution of superior HEA composites reinforced with sustainable materials for various engineering applications, by effectively combining computational predictions and experimental validation methods.

Keywords: High-Entropy Alloys (HEAs); Coconut Shell Pyrolysed (CSP); Phase prediction; Machine Learning; Powder Metallurgy; Spark Plasma Sintering.

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Ultrathin MOF Nanosheets and their Mixed-Matrix Membranes for Ammonia and Aliphatic Amines Sensing in Water

Ritu ladhi, Arshminder Kaur Dhillon, Monika Singh*

Institute of Nano Science and Technology (INST), SAS Nagar (Mohali), India.

*Corresponding Author E-mail: monika@inst.ac.in

ABSTRACT

Ultrathin 2D metal-organic frameworks (MOFs) possess a wide range of unique properties, making them highly suitable for diverse applications. However, creating a 2D MOF sensor capable of detecting hazardous amines in water has been a significant challenge. To address this issue, we synthesized Ni-*btc* MOF ultrathin nanosheets with a thickness of approximately 4.15 nm for the detection of amines in water. These nanosheets showed a remarkable "turn-on" fluorescence response when exposed to ammonia and aliphatic amines. The detection limit for aliphatic amines ranged from 297 to 424 nM, while for ammonia, it reached an impressive low limit of around 42 nM, an excellent value compared to other MOF-based sensors for ammonia sensing in water. Density functional theory calculations elucidated the mechanism underlying fluorescence enhancement. Additionally, a mixed matrix membrane based on MOF nanosheets was fabricated for real-time sensing that exhibits an immediate color change in the presence of ammonia and aliphatic amines.

Keywords: Metal-organic framework (MOF); Mixed matrix membrane (MMM); Fluorescence.

References

1. R. Ladhi, A. K. Dhillon and M. Singh, Ultrathin MOF nanosheets and their mixed-matrix membranes for ammonia and aliphatic amine sensing in water, *Nanoscale*, **2024**, 16, 8836-8842.

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Laser-Induced Crafting of Modulated Structural Defects in MOF-Based Supercapacitor for Energy Storage Application

Aashi, Rekha Rani, Srinivasan Alagar, Jatin Sharma, Arun K, Vivek Bagchi*

Energy and Environment Research Lab, Institute of Nano Science and Technology, Sector -81, Knowledge City, Sahibzada Ajit Singh Nagar- 140306, Punjab, India.

*Corresponding Author Email: bagchiv@inst.ac.in

ABSTRACT

Metal-organic frameworks (MOFs) have emerged as promising contenders in storage applications due to their unique properties. In this study, we synthesized CuZn-MOF-P_x by meticulously adjusting laser power during fabrication. This precise tuning substantially enhanced controlled defects and porosity, enhancing the electrode's surface area and specific capacitance. The optimized CuZn-MOF-P_7 electrode demonstrated a specific capacitance of 3.7 F cm^{-2} at 1 mA cm^{-2} of current density. Furthermore, the electrode showed outstanding durability, holding onto 97% of its capacitance at 50 mA cm^{-2} after 16000 cycles. To demonstrate its practical utility, we engineered a planar hybrid supercapacitor (PHSC) employing CuZn-MOF-P_7 as the cathode and activated carbon (AC) as the anode. This configuration displayed 22.3 µWh cm^{-2} and 6.75 mW cm^{-2} of energy and power density, respectively, highlighting its efficiency and applicability. This work's significance lies in the innovative use of a laser-irradiated approach for improving the performance of MOF-based materials for energy storage devices.

Keywords: Laser radiation; Planer hybrid supercapacitor; Structural defects; Diffusion coefficient.

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Influence of Process Parameters and Heat Treatment on the Fatigue Performance of Inconel 718 Fabricated through Selective Laser Melting

Arun B S[1], Anand Sekhar R[1,*], Ajukumar V N[2]

[1]*Department of Mechanical Engineering, TKM College of Engineering, Kollam 691005, Kerala, India.*

[2]*APJ Abdul Kalam Technological University, Thiruvananthapuram, Kerala, India.*

*Corresponding Author E-mail: anand@tkmce.ac.in

ABSTRACT

Many critical process parameters affect the fatigue performance of super alloys produced by Selective Laser Melting (SLM). These parameters affect the microstructure, surface roughness, and defect formation and play a significant role on the fatigue life of the super alloys. Optimizing these parameters in combination with appropriate post-processing techniques is crucial to extending fatigue life by decreasing defects. In the present work two set of Inconel718 (IN718) samples were prepared under two different energy densities. According to ASTM E606, a low cycle fatigue test is conducted to assess fatigue performance. Samples with lower energy density showed better fatigue life (Nf) of 858 number of cycles under strain amplitude of 0.8% and the corresponding stress amplitude is 866 MPa. Solution plus Single Aging heat treatment (HT) is adopted to dissolve the brittle lave phase and precipitates γ and γ′ phases to enhance the microstructure of alloy. Selective laser melted IN718 have unique microstructure due to the quick solidification and frequent thermal cycling involved in the process. In order to investigate the microstructure and metallurgical evolution, Optical microscopy (OM), Scanning electron microscopy (SEM), X-ray diffraction analysis (XRD), and Energy-dispersive X-ray spectroscopy (EDS) analysis were carried out. OM images showed equiaxed grains compared to coarse columnar crystals in as-built counter parts. Back scattered electron images showed the presence of δ phase in grain boundaries in addition to some irregular laves phases. X ray diffraction study identify the fcc structures (γ, γ′) and corresponding lattice planes. The present study establishes a relationship with process parameters, heat treatment and fatigue properties of selective laser melted IN718.

Keywords: Selective Laser Melting; Process parameters; Inconel718; Fatigue life; Microstructure.

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Machine Learning enabled Tribological Studies of Aerospace Materials

Vinayak P[1], Arun B S[2], Abhijith R[1], Stervin X[1], Suryanarayanan C S[1], Anand Sekhar R[1,*]

[1]*Department of Mechanical Engineering, TKM College of Engineering, Kollam 691005, Kerala, India*

[2]*Department of Mechanical Engineering, College of Engineering Trivandrum, Thiruvananthapuram 695016, Kerala, India*

*Corresponding Author E-mail: anand@tkmce.ac.in

ABSTRACT

Additive Manufacturing (AM) has revolutionized the manufacturing industry, producing complex, high-performance components with customized properties. Aerospace materials are subjected to extreme operational environments, exhibiting exceptional mechanical properties, including high strength to weight ratio, high wear resistance, low friction, etc. This study investigates the tribological behaviour of Ti-6Al-4V, a critical alloy in the aerospace industry, fabricated with optimized wear properties through Selective Laser Melting (SLM) technology, a Laser-Based Additive Manufacturing (LBAM) technique. The microstructure of AM-ed alloy has a significant impact on the required mechanical properties. Microstructure of the fabricated alloy varies with respect to the SLM process parameters such as Scanning speed, Laser power, Hatch spacing, Layer thickness, etc. Hence the process parameters of the SLM can be optimized for a better microstructure, which ultimately will result in better mechanical properties. Machine Learning models like Random Forest Regression (RFR), XGBoost and Support Vector Regressor (SVR), were used to predict wear properties and further optimize the process parameters, thereby obtaining samples of better wear characteristics. The requirement of ML models like RFR, XGBoost, and SVR is necessary for this study because of their ability to model complex, nonlinear relationships in the AM process, optimize multiple objectives, predict wear properties with high accuracy, and handle large, complex datasets. These models significantly reduce the need for time-consuming experimental trials and offer better control over process parameters, resulting in the production of high-performance components with superior wear characteristics. The XGBoost model stood out amongst other models, yielding an R^2 value of 0.963. Also detailed microstructural analysis justify the change in property values under different loading conditions, sliding speeds, and environmental settings, in doing so simulating real-world applications. Moreover, this study can be a useful reference, regarding the performance of AM-ed Ti-6Al-4V in wear critical environments, contributing to broader understanding of its potential in various engineering applications.

Keywords: Selective Laser Melting (SLM); Ti-6Al-4V; Machine Learning; Tribological Behaviour.

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Synergistic Modulation in a Triphasic Ni_5P_4-Ni_2P@Ni_3S_2 System Manifests Remarkable Overall Water Splitting

Vikas Pundir, Ashish Gaur, Rajdeep Kaur, Jatin Sharma, Rajinder Kumar and Vivek Bagchi*

Institute of Nano Science and Technology, Sector-81, Knowledge City, Sahibzada Ajit Singh Nagar, Punjab, 140306, INDIA

* Corresponding author E-mail: bagchiv@inst.ac.in

ABSTRACT

The potential for water splitting electrocatalysts with high efficiency paves the way for a sustainable future in hydrogen energy. However, this task is challenging due to the sluggish kinetics of the oxygen evolution reaction (OER), which has a significant impact on the hydrogen evolution process (HER). Herein multi-heterointerface of Ni_5P_4-Ni_2P@Ni_3S_2 was fabricated by a two-step synthesis procedure that consist the development of Ni_5P_4-Ni_2P nanosheets over nickel foam followed by the electrodeposition of Ni_3S_2. The HR-TEM analysis shows that the Ni_5P_4-Ni_2P@Ni_3S_2 nanosheets array provide numerous well-exposed diverse heterointerfaces. The electrochemical investigations conducted on the Ni_5P_4-Ni_2P@Ni_3S_2 nanosheets for complete water splitting indicate that they possess an overpotential of 73 mV and 230 mV in HER and OER respectively, enabling them to generate a current density of 10 and 50 mA cm^{-2}. The nanosheets also demonstrate Tafel slope values of 95 mV dec^{-1} and 83 mV dec^{-1} for HER and OER, respectively. The HER stability of the catalyst was conducted for 45 hours using chronoamperometric technique under a current density of 20 mA cm^{-1}, while the stability test for OER was carried out at current densities of 100 and 200 mA cm^{-1} for 100 hours each. Furthermore, in the overall water splitting, the catalyst exhibits a cell voltage of 1.47 V@10 mA cm^{-2} and displayed a stability operation for 100 hours at a current density of 150 mA cm^{-1}.

Keywords: Hydrogen evolution reaction; Electrocatalyst; Nickel sulfide; Nickel phosphide; oxygen evolution reaction.

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Review on Gravitational energy storage

J sharukesh[1,*], S Arun prakash[1], M Prithivi raj[2]

[1]*UG, Second Year Students, Department of Mechanical Engineering, Kamaraj College of Engineering and Technology, Virudhunagar.*

[2] *Assistant Professor, Department of Mechanical Engineering, Kamaraj College of Engineering and Technology, Virudhunagar.*

*Corresponding Author E-mail: skesh0111@gmail.com

ABSTRACT

As the demand for sustainable energy solutions rises, innovative energy storage technologies are gaining popularity. Gravitational potential energy storage transforms energy into electrical energy using fundamental physics concepts. By employing surplus energy from renewable sources (wind and solar) to raise heavy items, GES systems offer an innovative approach to energy storage that addresses the shortcomings of traditional battery technology. In order to raise a mass which could be water, solid weights, or other materials to a certain height, GES need additional energy. When energy demand increases or renewable generation declines, the mass's stored energy is converted back into electricity to power a generator. This process can be thought of as a reversible energy transformation that takes advantage of gravity. GES's excellent energy efficiency is one of its key advantages. Efficiency ratings of most GES systems are on par with or better than those of traditional energy storage technologies. The lifting mechanism's design, the kind of mass being used, and the generator's parameters are some of the variables that affect efficiency. There are several different types of GES systems, including vertical towers and underground installations. These solutions can lessen the need for new development and its detrimental effects on the environment by merging with existing infrastructures. GES's scalability, which enables systems to be deployed at different scales—from modest community projects to massive utility installations—is another important advantage. GES's versatility allows it to satisfy a variety of energy requirements in various settings. In contrast to traditional batteries, which frequently use rare earth elements and have short lifespans, GES systems don't deteriorate over time and have little adverse environmental impact. GES's robustness makes it a more environmentally beneficial choice for long-term energy storage because it requires fewer replacements and generates less trash. Maintaining grid energy balance requires GES systems, particularly when including intermittent renewable energy sources. GES can improve grid stability and resilience by offering a dependable way to store and distribute energy. Geospatial Energy Management (GES) is a promising answer to the problems of energy variations and supply-demand imbalances as global infrastructure moves toward a more renewable energy-focused strategy.

Keywords: Gravitational energy storage; Renewable energy; Energy efficiency; Grid stability.

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Analysis of Stress Fields Near Grain Boundaries During Micropillar Compression Testing in Ni-Based Superalloys

Manmath Kumar Dash[1*], Longfangdi Shi[2], Yu-Lung Chiu[2]

[1]*Department of Materials and Metallurgical Engineering, Maulana Azad National Institute of Technology, Bhopal, Madhya Pradesh, India, 462003*
[2]*School of Metallurgy and Materials, University of Birmingham, Birmingham, UK, B15 2TT*
*Corresponding Author E-mail: manmathd@gmail.com

ABSTRACT

Grain boundaries exert a critical influence on the mechanical behaviour of polycrystalline materials by impeding dislocation glide and governing deformation mechanisms. During mechanical loading, dislocation pile-ups at grain boundary interfaces induce stress concentration, leading to inhomogeneous stress distributions that contribute to local stress fields and microscale damage nucleation. This study aims to quantify the stress fields near grain boundaries in Ni-based superalloys under micropillar compression, utilizing in-situ high-angular resolution electron backscatter diffraction (HR-EBSD) to elucidate the deformation constraints imposed by the boundary interface. Micropillar compression tests were performed on Ni-based superalloys under varying strain conditions to delineate the elastic and plastic regions adjacent to grain boundaries. The grain boundary interface plane was oriented approximately perpendicular to the loading axis to ensure a uniform stress distribution during testing. Initial electron backscatter diffraction (EBSD) analysis revealed a macroscopically straight grain boundary, contrasting with a corrugated structure at the microscopic scale. Quantitative stress field analysis demonstrated that localized variations in grain boundary curvature critically influenced slip transfer resistance, resulting in heterogeneous mechanical strength across the boundary. Furthermore, increased plastic strain promoted stress-driven grain boundary migration. The local stress distribution across the grain boundary interface was further rationalized through 3-dimensional subsurface analysis, providing insights into boundary inclination and its role in stress accommodation.

Keywords: Local stress; Grain boundary; EBSD, Micropillar compression.

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Adsorption Study of Activated Biochar Derived from the Ficus Auriculata Tree Leaves on Anionic and Cationic Dyes

Divya D, Binitta K , Shijo Thomas*

Department of Materials Science and Engineering, NIT Calicut, India

*Corresponding Author E-mail: shijo@nitc.ac.in

ABSTRACT

Access to clean water is a fundamental requirement for human health and holistic well-being. Textile dyes are a major source of water pollution, and their treatment is necessary to safeguard the environment. Several viable methods exist for eliminating dyes from wastewater. The high adsorption efficiency for dye removal has positioned this method as a perfect substitute for more costly treatment techniques. This study used activated biochar from the pyrolysis of the Ficus auriculata tree leaves as the adsorbent. A two-step method was used to prepare the activated biochar. The biochar was first pyrolysed at 800ºC and then was KOH activated. The prepared adsorbent was characterised by Fourier transform infrared spectrometry (FTIR), thermogravimetric analysis (TGA), scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX), X-ray diffractometry (XRD), and Brunauer-Emmett-Teller model (BET). The results showed that the activated biochar has a mesoporous structure with a high surface area (2102.6 m^2/g) and possesses abundant active groups on the surface, further enhancing the adsorption efficiencies. Cationic (methylene blue) and anionic (methyl orange) organic dyes were used to study the adsorption mechanism of the activated biochar. Batch adsorption studies were carried out. The equilibrium data of different concentrations were analysed using Langmuir and Freundlich's isothermal models. The kinetic studies were carried out with the first- and second-order pseudo-reaction equations. Overall, Activated biochar from Ficus auriculata leaves has excellent adsorption potential for cationic and anionic dyes; therefore, they can be considered a cost-effective and efficient adsorbent.

Keywords: Activated Biochar; Ficus auriculata leaves; Organic dyes; Adsorption; Isotherms.

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Machine Learning Enabled Exploration of Tensile Traits of Aerospace Material Fabricated by SLM Technology

Muhammed Nazim N[1], Arun B S[2], Faris Sidhikhu[1], Rehan Anil[1], Bhagyanath M Krishna[1], Anand Sekhar R[1,*]

[1]*Department of Mechanical Engineering, TKM College of Engineering, Kollam 691005, Kerala, India*

[2]*Department of Mechanical Engineering, College of Engineering Trivandrum, Thiruvananthapuram 695016, Kerala, India*

*Corresponding Author E-mail: anand@tkmce.ac.in

ABSTRACT

Additive manufacturing (AM) of aerospace materials is getting wider attention, and the properties of AM samples are widely different from conventional alloys because of the variation in the AM process parameters. In this study, the trained machine learning models like Decision tree, Gradient boosting, and Multivariable linear regression were used to predict the significant process parameters for better tensile traits. The requirement of ML models is necessary for this study, because of their ability to model complex, nonlinear relationships in the AM process, predict properties with high accuracy, and handle large, complex datasets. As a result, the Inconel 718 (IN718) samples with superior tensile properties were fabricated by the AM process. The AM-ed Inconel 718 samples shows better strength, ductility, and hardness in the tensile tests conducted on a Computerized Universal Testing Machine (UTM). The detailed microstructural analysis reveals a better microstructure, layers and grain structure created during fabrication. This work significantly contributes to the aerospace industry for producing reliable, high-performance IN718 components in demanding environments.

Keywords: Selective Laser Melting (SLM); Inconel 718; Machine Learning; Tensile properties.

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Thermal Performance Enhancement of Natural Fibre Reinforced Recycled Polystyrene Composite through Material Optimisation and Pore Structure

M Krishnaprasad Varma, Bijo Abraham Jacob, Sudhanshu Nartam, Ummen Sabu ,

S Budhe*

Department of Mechanical Engineering, National Institute of Technology Calicut, NIT Campus P.O- 673601, Kozhikode, Kerala, India

*Corresponding Author E-mail: sandip@nitc.ac.in

ABSTRACT

The packaging industry is producing large amounts of thermocol waste every year and recycling of these waste materials is essential for sustainability. Application of thermocol to fabricate the composite materials can be used to provide thermal insulation which helps to reduce the domestic carbon footprint (in households). The main aim of this research work is to optimize the weight ratio of natural fibre and filler materials in bamboo fibre reinforced recycled polystyrene matrix composite to minimize the thermal conductivity. Unwoven bamboo fibres pre-treated with hydrogen peroxide are mixed with a solution of polystyrene (recycled thermocol) in acetone and ethyl acetate mixture. Pore forming agent added to enhance the air pore in the composite material which may lead to better insulation. Thermal conductivity analysis is done for different weight ratios of the composites using hot disk method. Hot disk TPS 500S is used to measure the thermal conductivity at various conditions. The porosity of samples is analysed using Scanning Electron Microscopy (SEM). There is a decreasing trend in thermal conductivity of the sample with the higher percentage of thermocol and pore in composite. Pore forming agents further increase porosity and decrease conductivity. Thermal conductivity is showing a decreasing trend with increase in pores. The samples are found to have lower thermal conductivity compared to concrete making them useful in thermal insulation of the buildings. Wall tiles manufactured using this composite material can be used to reduce the energy demand of buildings. The use of this composite material as a noise damper owing to its porous nature should be further analysed for various other applications.

Keywords: Thermocol; Recycling; Sustainability; Composite Materials; Thermal conductivity.

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Development and Characterization Of Electrospun Pva Nanofibrous Scaffold Incorporated with Green Synthesized Copper Oxide Nanoparticles And Curcumin for Wound Healing Applications

Kawshik S[1], Nithin S N[2], Lamiya Nasreena[2], Hanas T[2,*]
[1]*Department of Biotechnology, Bannari Amman Institute of Technology*

[2]*Department of Materials Science, National Institute of Technology Calicut*

*Corresponding Author E-mail: hanas@nitc.ac.in

ABSTRACT

Polyvinyl alcohol (PVA) nanofibers incorporated with green synthesized copper oxide nanoparticles (CuO NPs) and nano curcumin targeted for wound healing applications were developed by electrospinning technique. applications. The performance of the developed samples was compared with scaffolds incorporated with chemically synthesized nanoparticles. Scanning Electron Microscopy (SEM) confirmed the nanoscale size of the particles and their distribution in the fibres, while X-ray Diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR) characterized the crystalline structure and functional groups present in the samples. The water contact angle confirmed that the incorporation of the synthesized nanoparticles did not affect the hydrophilic nature of electrospun fibres which is crucial for chronic wound healing. Mechanical testing revealed that the incorporation of nanoparticles and crosslinking increased the mechanical strength of the nanofibers. The wound healing efficacy of green synthesized nanoparticles was compared with chemically synthesized ones through biological studies, including antioxidant activity, MTT assay, wound scratch assay, and antibacterial studies. The tests confirmed that green synthesized nanoparticles are equally effective in antibacterial and antioxidant activity while demonstrating higher biocompatibility and faster wound healing. It is proposed that curcumin and green synthesized CuO NP-incorporated PVA nanofibers can provide a robust, biocompatible scaffold with superior wound-healing potential compared to chemically synthesized counterparts.

Keywords: Electrospinning; Green NPs; Curcumin; Antibacterial; Wound healing.

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Microstructural Evolution and Its Impact on Mechanical Properties of INCONEL 600 under Thermomechanical Treatments

Ruttala Naidu, Manmath Kumar Dash*

[1]*Department of Materials and Metallurgical Engineering, Maulana Azad National Institute of Technology, Bhopal, Madhya Pradesh, India, 462003*

*Corresponding Author E-mail: manmathd@gmail.com

ABSTRACT

INCONEL 600 is extensively employed across various industries due to its remarkable resistance to both corrosion and elevated temperatures. The alloy's superior high-temperature performance and extended service life are largely attributed to its stable single-phase microstructure, which remains intact up to 1703 K (1430 °C). In this study, the microstructural evolution of INCONEL Alloy 600 was systematically examined under a range of thermal and thermomechanical treatments. These microstructural analyses were complemented by mechanical property assessments, including tensile and creep tests. Specimens were solutionized at 1200 ºC for 1 hour, resulting in a microstructure characterized by an average grain size distribution between 45-60 µm. Additionally, primary and secondary carbides rich in Cr, Nb, and Ti were observed within the γ matrix. The alloy was subsequently subjected to cold forging at room temperature, with varying levels of strain ranging from 20% to 50%, followed by post-deformation heat treatments. Microstructural features were analysed using advanced electron microscopy techniques, while nanoindentation tests were employed to investigate indentation load-depth profiles at a finer scale, providing insight into localized mechanical behaviour. Furthermore, analytical modelling was conducted to elucidate the micromechanisms governing plastic deformation, with a particular focus on the role of microstructural attributes, such as dislocation density and carbide distribution, in influencing the plasticity of the alloy.

Keywords: INCONEL 600; Thermomechanical Treatment; Microstructural Engineering.

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Investigation of Size-Dependent Plasticity in Nickel-Based Superalloys

Chintapatla Tirumala Surya Prakash, Manmath Kumar Dash*

Department of Materials and Metallurgical Engineering, Maulana Azad National Institute of Technology, Bhopal, Madhya Pradesh, India, 462003

*Corresponding Author E-mail: manmathd@gmail.com

ABSTRACT

In the current scenario, there is significant interest in fabricating small structures for a wide range of applications. Nickel-based superalloys have emerged as a material with proven applications in the aerospace industry, particularly for rocket engine components. Their use is now extending to microscale devices, where they interact at the micro-scale and even nanoscale, leading to complex contact-induced deformations that require detailed attention. Size-dependent plasticity, observable from the micron to nanoscale, necessitates considering size effects in nano-regimes. This study incorporates various continuum theories to account for size effects across different length scales in plasticity. In current study, the load vs. displacement (L-D) curves is utilized from nano-indentation tests conducted at different loads (2 mN, 5 mN, and 10 mN) to establish the size effect within the microstructure. Initially, the L-D curves exhibited similar trends and nearly comparable slopes across the given loads. However, variations in hardness were observed with changing loading conditions, showing a decrease in hardness as the load increased. This finding supports the development of strain gradient plasticity theory and its application to understanding size-dependent hardness variations from the micro- to nanoscales.

Keywords: Size-dependent plasticity; Nano-indentation; Analytical modelling.

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Evaluation of Chitosan Scaffolds for Bone Regeneration in Post-Extraction Sockets: A Clinical Study

Aswathi Vinod[1,2], Aparna Zagabathuni[1, *],Manoj Kumar K.P[2],Sunu V S[2] ,Mohammed Afsar[2], Dhanya Muralidharan[2]

[1]*Department of Materials Science and Engineering, National Institute of Technology Calicut, Calicut, Kerala, India*

[2]*Department of Oral and Maxillofacial Surgery, KMCT Dental College, Manasery, Kerala, India*

*Corresponding Author E-mail:aparnazagabathuni@nitc.ac.in

ABSTRACT

Chitosan has emerged as a promising material in tissue engineering due to its biocompatibility, biodegradability, hemostatic and osteoconductive properties. This study aimed to assess the efficacy of chitosan scaffolds for bone regeneration in post-extraction sockets, leveraging its potential for promoting osteoblast differentiation and reducing inflammation. The structural and chemical integrity of the chitosan scaffold was carried out by X-ray diffraction (XRD), Scanning electron microscopy (SEM), and Fourier-transform infrared spectroscopy (FTIR). Twenty patients undergoing dental extractions at KMCT Dental College were selected. The test group received chitosan scaffold placement, while the control group underwent standard care. Clinical and radiographic evaluations of soft and hard tissue healing were performed. In the test group, 15 out of 20 patients exhibited superior bone regeneration compared to the control group. One patient showed reduced healing, and four showed significant differences between the groups. Chitosan facilitated enhanced osteoblastic and cementoblastic activity, improving bone and cementum formation. The findings suggest that chitosan scaffolds are effective in enhancing hemostasis & bone regeneration in dental applications, particularly in post-extraction sockets.

Keywords: Chitosan; Biodegradable; Osteoconductive;, Hemostasis; Post-extraction healing.

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Preparation of Eco-Friendly Fireworks Composition with Corncob Powder to Reduce SO_2 Emission

S Hari Prasad, P V Deepthika, J Midunprasanth, N Manikandan,

M Surya Prakash Kumar, S Shanthini, T Hari Prasath*

Department of Electrical and Electronics Engineering, Kamaraj College of Engineering and Technology, Virudhunagar, India

*Corresponding Author E-mail: hariprasad54046@gmail.com

ABSTRACT

Firework products are commonly used by people during festival times. There are various types of fireworks like crackers, rockets, flowerpots etc. which can be used during day and night time. Normally crackers are made of flash powder composition which comprises of aluminium, potassium nitrate and sulphur. In general sulphur is present in all firework composition due to its excellent thermal property. Sulphur is used as it lowers the temperature required to ignite the mixture. Though sulphur being an integral component in firework composition, the ability of sulphur to form sulphur dioxide as a by-product of combustion is a major consent. The use of sulphur must be reduced with an alternative material in order to control the emission of SO_2 in the atmosphere. This could be replaced with a combustible material like corncob powder, because the corncob powder has lower sulphur. When oxidised, it forms only less amount of SO_2 and they are often used as a biomass fuel because they burn relatively efficiently and produce a good amount of heat. This novel work is carried out by reducing sulphur in various proportion along with the inclusion of corncob powder.

Keywords: Sulphur Reduction; Corncob Powder; Firework Composition; Sulfur Dioxide (SO_2) Emissions; Biomass Fuel.

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Enhancing the Mechanical Properties of Recycled PLA-TPU Blends through Polymer Blending Using a Twin-Screw Extruder and Compatibilizer Addition

M Krishnaprasad Varma*, **Mallavarapu Prudhvi**, Aditya Bhosale, Ansif Jameel C M , Sharu B K

Department of Mechanical Engineering, National Institute of Technology Calicut, NIT Campus PO-673601, Kozhikode, India

*Corresponding Author E-mail: varma_b211104me@nitc.ac.in

ABSTRACT

The integration of additive manufacturing with polymer recycling is a very efficient method to enhance the value of waste, a practice that was previously condemned.The increasing need for sustainable materials as alternatives to traditional materials has created a requirement for sustainable manufacturing methods that can efficiently counterbalance the utilization of finite resources and minimize environmental consequences, all while ensuring economic feasibility and advancing human well-being. Efficient recycling of 3D-printed PLA is essential for minimizing carbon emissions during production and promoting circular economy principles. However, regenerated PLA filaments generally have reduced mechanical strength and thermal stability, which can be problematic for additive manufacturing applications. This study explores the development of sustainable, high-performance PLA-TPU composites for soft robotics by utilizing recycled PLA. By optimizing the PLA-TPU weight ratio and incorporating a compatibilizer, we sought to enhance key mechanical properties such as tensile strength, impact resistance, and flexural fatigue strength. The composites were fabricated using a twin-screw extruder and injection molding process, and the mechanical performance was evaluated according to ASTM standards. Morphological analysis via scanning electron microscopy revealed detailed insights into the polymer microstructure and phase interactions within the composites. The findings indicate that TPU significantly improves the mechanical properties of recycled PLA, making it a promising candidate for soft robotic applications requiring elastomers with high tensile strength. However, the long-term durability and environmental impact of these composites need further investigation.

Keywords: Polymer Recycling; PLA-TPU Composites; Sustainable Materials; Mechanical Properties.

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Optimization of Densification Process and Microstructure of Cold Isostatic Pressed (CIP) 18Cr-ODS Ferritic Steel Powder

T Siva Kumar Prudhvi Raj[1], Manmath Kumar Dash[2,*]

[1]*Metallurgical and Materials Engineering, Rajiv Gandhi University of Knowledge Technologies, Nuzvid, Andhra Pradesh, India, 521202*
[2]*Department of Materials and Metallurgical Engineering, Maulana Azad National Institute of Technology, Bhopal, Madhya Pradesh, India, 462003*
*Corresponding Author E-mail: manmathd@gmail.com

ABSTRACT

This study examines how 18Cr ODS ferritic steel behaves during sintering under different conditions, like temperatures from 1050 ºC to 1250 ºC and atmospheres of Air, Hydrogen, and Argon. It assesses density, microstructure, and microhardness of the sintered samples to understand the effects of these factors on material properties. Results show that sintering in a Hydrogen atmosphere consistently produces the highest density, thanks to its ability to prevent oxidation and reduce oxide layers on powder particles. Density increases with temperature until 1150 ºC, after which grain coarsening becomes more prominent. The optimal conditions for compaction (92% density) and a uniform microstructure were achieved at 1150 ºC for 2 hours in a Hydrogen atmosphere. Overall, this study offers valuable insights into optimizing sintering parameters for 18Cr ODS ferritic steel, with potential benefits for enhancing material properties and performance in various applications.

Keywords: ODS Steel; Powder Metallurgy; Sintering.

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Effect of Annealing on the Physical properties of Electron Beam Evaporated Vanadium Oxide Thin Films

K V Madhuri[1,*], Y V Omprakash[1]

Department of Physics, Thin Film Research Centre, Vignan's Foundation for Science Technology & Research (Deemed to be University), Vadlamudi, Guntur, Andhra Pradesh, India 522213

*Corresponding Author E-mail: kvmsvu@gmail.com

ABSTRACT

Researchers have been interested in vanadium oxides among the other transition metal oxides because of their multiple valency and existence in both stoichiometric and sub-stoichiometric states. Among these, the semiconducting disordered metamaterial V_2O_5 has the highest stability and oxidation level. V_2O_5 in thin film form, plays a crucial role in gas sensors, smart windows, microelectronic devices, chromogenic and switching devices, and gas sensors because of its layered structure and metal-insulator transition. In the present work, V_2O_5 thin films are fabricated by e-beam evaporation onto the well-cleaned glass substrates. The thickness of the films was controlled by an inbuilt quartz thickness monitor. The color of freshly evaporated V_2O_5 thin films was found to be yellow, and the films were poorly adherent to the surface. To improve the adherence, the substrate temperature was increased to 200^{o}C. Hence the color of the films changed from pale yellow to orange yellow. With the increase in substrate temperature, the films indicate the sub stoichiometry. To overcome this, the films were annealed at 200, 300 and 400℃ for 1 hour and obtained uniform and pinhole-free films. The experimental films undergo systematic characterization for their structural and optical properties. X-ray diffraction studies reveal that the deposited films are crystalline in nature, which was improved by annealing. The annealing process helped in the formation of well-defined crystalline phases and also enhanced the structural order. The films showed various mixed phases. Structural properties revealed that the films are uniform and becoming dense with annealing temperature. EDS proved the elemental concentration of vanadium and oxygen in these V_2O_5 thin films. The optical transmittance spectra revealed that the films exhibit a direct forbidden transition. The variation in the optical properties due to annealing is more pronounced for chromogenic applications.

Keywords: V_2O_5 thin films; Electron beam evaporation; Structural and Optical properties.

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The role of annealing on structural, mechanical and tribological properties of 3D printed PLA/ Pyrolytic carbon composite

Vivek C Ravi, Aparna Zagabathuni*

Department of Materials Science and Engineering, National Institute of Technology Calicut, Calicut, Kerala, India

*Corresponding Author E-mail: aparnazagabathuni@nitc.ac.in

ABSTRACT

Polylactic acid (PLA) is a popularly used biopolymer known for its environmentally sustainable and biodegradable characteristics; however, its mechanical properties limit its application in various medical applications. To address this and to enhance the tribo-mechanical performance of PLA, renowned biocompatible material, pyrolytic carbon (PYC) is integrated. In this study, three different concentrations of PYC (0.5 wt.%, 1 wt.%, and 1.5 wt.%) were incorporated into commercially available PLA resin and the components were fabricated using SLA 3D printer. The resulting nanocomposites were structurally characterized using X-ray diffraction (XRD) and Scanning electron microscopy (SEM). Tensile testing demonstrated that PLA exhibited superior performance, exceeding the 0.5 wt.% and 1.5 wt.% composites by 50%, attributed to poor interfacial adhesion between PYC and PLA. To enhance the interfacial bonding both between layers and between PYC and PLA, the specimens were annealed at 90 °C for a duration of 120 minutes. The research demonstrated that the annealing process substantially improved the tensile strength, young's modulus, toughness, and tribological properties of the specimens, especially when the reinforcement concentration was up to 1 wt.%. However, these properties began to deteriorate beyond this concentration level. The improved mechanical properties were ascribed to higher crystallinity and stronger interfacial adhesion between the PLA matric and pyrolytic carbon particles. This study highlights the critical balance between reinforcement concentration and processing conditions, suggesting that optimal annealing can lead to superior performance in 3D printed composites, making them suitable for a variety of applications.

Keywords : Annealing; 3D printing; Polylactic acid; Pyrolytic carbon.

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Development of Ionic Fluid for Photocatalytic Reduction of CO_2

Jayash Sahu[1], Shijo Thomas*

Department of Materials Science and Engineering, National Institute of Technology Calicut, Kerala, India

*Corresponding Author E-mail: jayash_b210968mt@nitc.ac.in

ABSTRACT

This study focuses on the development and characterization of ionic fluids, specifically 1-butyl-3-methylimidazolium acetate ([Bmim][Ac]), for integrating advanced nanomaterials in photocatalytic systems. The work centers on synthesizing and optimizing Tubular Graphitic Carbon Nitride (TGCN) and Graphitic Carbon Nitride Nanofibers (GCNNF) to enhance their photocatalytic properties. The research investigates the effects of varying dopant concentrations on TGCN, analyzing structural and electronic properties using advanced characterization techniques. Among the synthesized variants, mildly doped TGCN demonstrated superior photocatalytic performance compared to low- and high-doped samples. This improvement is attributed to better charge separation and light absorption, crucial for photocatalytic applications. The experiments were conducted under ambient conditions and visible light, ensuring that the results are applicable to real-world scenarios. The ionic fluid [Bmim][Ac] was acting as a reactive medium for CO_2 absorption, facilitating their uniform interaction with light and reactants. While this study does not directly address CO_2 capture or reduction, the findings provide valuable insights into material behavior, laying the groundwork for future applications in carbon mitigation technologies. This work establishes a robust foundation for the development of photocatalytic systems. The optimized performance of doped TGCN under visible light presents promising implications for sustainable energy and environmental applications. The findings will serve as a basis for future research into integrating these materials with ionic fluids for CO_2 capture and conversion technologies.

Keywords: Ionic fluid; Photocatalysis; Graphitic Carbon Nitride.

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Sono-Photo-Fenton Degradation of Organic Pollutants Using MoS_2–$MnFe_2O_4$ Heterojunction

Vishakha Takhar[1], Simranjit Singh[2], Rupak Banerjee[1,3*]

[1]*Department of Physics, Indian Institute of Technology Gandhinagar, Palaj, Gandhinagar - 382355, India*

[2]*Materials Engineering, Indian Institute of Technology Gandhinagar, Palaj, Gandhinagar - 382355, India*

[3]*K C Patel Centre for Sustainable Development, Indian Institute of Technology Gandhinagar, Palaj, Gandhinagar - 382355, India*

*Corresponding Author E-mail: rupakb@iitgn.ac.in

ABSTRACT

The generation of reactive oxygen species by nanomaterials offers a promising approach for the degradation of organic pollutants in water. This study demonstrates the reactive oxygen species generating properties of a composite made from MoS_2 nanosheets and $MnFe_2O_4$ nanoparticles. Electrochemical impedance spectroscopy revealed the formation of a type-II heterojunction, where MoS_2 functions as the electron donor and $MnFe_2O_4$ acts as the electron acceptor. Energy levels were constructed through ultraviolet photoelectron spectroscopy and band gap calculations. Morphological analysis using SEM and AFM showed MoS_2 nanosheets with a thickness of 0.6 nm and spherical $MnFe_2O_4$ nanoparticles with a size of around 5 nm. Detailed characterization of the heterojunction was performed using XRD, UV-Vis, FTIR, VSM, and XPS. The generation of reactive oxygen species by the composite was assessed by the degradation of methylene blue dye, with hydrogen peroxide, sonication, and visible light used as triggers for reactive oxygen species generation. Comparative analysis highlighted the superior performance of the composite under solo, dual, and triple trigger conditions compared to pristine $MnFe_2O_4$ and MoS_2. The composite exhibited a maximum dye degradation efficiency of 98% within 10 minutes of exposure under all triggers, significantly outperforming pristine MoS_2 at 45.5% and $MnFe_2O_4$ at 8%. Kinetic analysis revealed a pseudo-second-order reaction, with the composite showing the highest reaction rate. Reusability studies demonstrated that the composite maintained ~90% efficiency even after 10 cycles, and its magnetic properties allowed for easy recovery using an external magnet. The superior performance of the composite was further explained through scavenger experiments and electrochemical impedance spectroscopy measurements, which showed that efficient charge transfer between MoS_2 and $MnFe_2O_4$ reduces charge recombination, resulting in enhanced catalytic performance.

Keywords: Heterojunction; 2D material; Magnetic nanoparticles; ROS generation; Dye degradation.

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Biowaste Derived Electrocatalysts for Enhanced Direct Methanol Fuel Cell Performance: A Step Towards Sustainable Energy

Vanshika Sreekumar[1], Vishal Khandelwal[2,*]

Department of Materials Science and Engineering, National Institute of Technology Calicut, Calicut, Kerela, India

*Corresponding Author E-mail: vanshika_b210969mt@nitc.ac.in

ABSTRACT

For many decades, we have been using fossil fuels for energy production. However, recently, with a greater focus on decreasing the carbon footprint necessitates to switch to other viable alternatives like fuel cells became prudent. Direct Methanol Fuel Cells (DMFCs) are more widely used among the various fuel cells available, as they are hassle-free in terms of storage and transportation and hence attractive for use in portable applications. The two important reactions occurring in DMFC are the oxidation of the fuel methanol at the anode and the reduction of oxygen at the cathode, and they possess a suitable proton exchange membrane like the other proton exchange membrane fuel cells (PEMFC). The anode reaction involves the oxidation of methanol to carbon dioxide. In the cathode half of the cell, oxygen reduction takes place, which follows the $4e^-$ pathway *leading* to the formation of water. The presence of a thin membrane facilitates proton exchange and prevents the crossover of methanol from the anode to the cathode to ensure the normal functioning of the fuel cell, and prevents the scenario of over potential and decrease in the efficiency of the Fuel Cell. Using an active catalyst for ORR and MOR is necessary for DMFCs. As per the literature, Pt and Pt-based alloys are being extensively used as catalysts for ORR, but the high cost, poor stability, and poor methanol tolerance limit commercialisation. Hence the development of a catalyst from Biowaste is of great importance as it not only enhances the performance of the DMFC serving as a cost-effective green alternative to Pt-based catalysts but also when used as a catalyst support along with miniscule amount of active metals such as Ag, Mn it can serve as a more stable methanol tolerant catalyst with lower charge transfer resistance. It works as a clean and green energy conversion method. In the current research work, we utilised Biowaste of Green Moong Dal Beans and converted it into Biochar by pyrolysing it for 4 hrs at a temperature of 800°C. The obtained Biochar was tested for its electrochemical activity for ORR and it gave a performance of 4.5 mA/cm^2 which was a very good performance for a sample derived from Biochar. This catalyst support was seen to be highly active and selective material for ORR. Considering its activity the sample was doped with Silver Nanoparticles. Composite of Ag/Biochar was synthesized in the lab, which gave a current density of 5.5 mA/cm^2 which was much better as compared to the performance of Ag/C (Commercially used Vulcan Carbon) composite. The sample of Ag/Biochar showed repeatability and low charge transfer resistance as a catalyst in its performance. It also showed a much higher current density than Ag/C (Vulcan), as reported in the literature.

Keywords: ORR; MOR; Ag/C.

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Machine Learning Guided High Entropy Alloy Discovery: Accelerating Materials Innovation

Ridhin Raj V R, Aparna Zagabathuni*

Department of Materials Science and Engineering, National Institute of Technology Calicut, Kerala

*Corresponding Author E-mail: talk2ridhin@gmail.com

ABSTRACT

High-entropy alloys (HEAs) are a unique class of materials characterized by exceptional mechanical, thermal, and chemical properties, making them highly applicable in industries such as automotive, aerospace, and energy storage. However, the vast compositional space of HEAs presents significant challenges for efficient exploration using traditional methods. This work presents a novel approach that combines high-throughput techniques with machine learning (ML) to accelerate the HEA discovery process. The proposed model employs a deep neural network (DNN) to capture and forecast HEA characteristics, drawing from an extensive dataset of HEA properties such as strength, ductility, and resistance to corrosion. To address the wide compositional spectrum of HEAs, the model incorporates Bayesian optimization to focus on compositions that demonstrate the greatest compressive strengths. To gain deeper insights into the factors influencing HEA performance, feature importance analysis techniques like permutation importance and LIME (Local Interpretable Model-Agnostic Explanations) are applied. These methods help to identify the most critical elements and their interactions in determining the overall properties of HEAs. By combining these powerful techniques, this approach enables the rapid discovery and design of HEAs with tailored properties, significantly reducing the time and cost associated with traditional trial-and-error methods. This innovative methodology has the potential to revolutionize the development of advanced materials and accelerate the realization of next-generation technologies.

Keywords: High-entropy alloys; Deep Neural Network; Machine Learning.

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Magnetically Actuated Microbots for Efficient Biofilm Eradication

Vyom Bhalala, Abhimanyu B, Kartik Nehra, Abey Joseph, and Baiju G Nair

Department of Bioscience & Engineering, National Institute of Technology, Calicut, NIT Campus P.O 673 601, Kozhikode, India

*Corresponding Author E-mail: bgnair@nitc.ac.in

ABSTRACT

Marine biofouling, characterized by the persistent formation of biofilms on the surface of water vessels, results in severe operational inefficiencies, increased fuel consumption, and accelerated material degradation. This study introduces an innovative approach using magnetically actuated microbots designed for targeted biofilm eradication. The microbots are constructed with a structure composed of polymer, onto which MoS_2/Ag-TiO_2 (MAT NPs) are embedded. The polymer core offers biocompatibility and strong adhesion properties, while the MAT nanoparticles provide effective biofilm disruption and irradiation capabilities. Magnetic actuation is employed to control the movement and positioning of the microbots, allowing them to navigate through complex environments and target biofilms with high precision. The microbots demonstrate multimodal movement capabilities, enabling them to penetrate and disrupt the extracellular polymeric substances (EPS) matrix of the biofilms. This mechanical disruption, combined with the antimicrobial properties of the MAT NPs, results in significant biofilm eradication, reducing bacterial viability by over 99%.`

Keywords: Microbots; Marine anti-biofouling; Magnetic actuation; Polymer; MoS_2/Ag-TiO_2 nanoparticles.

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Numerical Investigation of Improved Efficiency of MoS_2 Based Solar Cell Using HTL And ETL

Sunita Tarei[1], Karan Dhuper[1,*], Siddhartha Duttagupta[2], Aswani Yella[3]

[1]*Centre for Research in Nanotechnology and Science (CRNTS), Indian Institute of Technology Bombay, Powai, Mumbai 400076, India*

[2]*Department of Electrical Engineering, Indian Institute of Technology Bombay, Powai, Mumbai 400076, India*

[3]*Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Powai, Mumbai 400076, India*

*Corresponding Author E-mail: kumar.karan058@gmail.com

ABSTRACT

The various studies have been done on 2D solar cell due to their distinctive optical and electrical characteristic. In addition, 2D transition metal dichalcogenides (TMDCs) have been utilized in solar cell structures in numerous studies. However, 2D solar cells exhibit low power conversion efficiency due to their absorption limitations. Therefore, Significant efforts have been devoted to enhancing the photovoltaic (PV) efficiency of thin-film solar cells (TFSC) by utilizing novel absorber materials with hole and electron transport layer. This study examines the performance of a solar cell structure comprising Molybdenum oxide (MoO_3), Tungsten disulphide (WS_2), and Tin oxide (SnO_2) using the one-dimensional Solar Cell Capacitance Simulator (SCAPS-1D) software. In this configuration, MoO_3, WS_2 and SnO_2 serves as the hole transport layer, active layer, and the electron transport layer, respectively. Further, this study investigates the impact of doping levels and thicknesses of the absorber and buffer layers on the performance parameters such as power conversion efficiency (PCE), filling factor (FF), short circuit current (I_{SC}) and open circuit voltage (V_{OC}). A significant enhancement in PCE and V_{OC} is found by incorporating the HTL in WS_2 solar cell. This effect prevails at a lower thickness of the WS_2 layer (0.1-1µm). Furthermore, the findings reveal the optimum value of doping concentration and defect density based on their performance parameters.

Keywords: TMDCs; Thin Film Solar cells; Hole Transport Layer; Electron Transport Layer; Efficiency; Performance Parameters; Recombination.

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Design and Analysis of a Novel Clamp Based Fixed-Ended Flexible Beam for Energy Harvesting from Sea Waves

Ishan Zalpuri[1], Dikshit Makwana [2], Aparna Zagabathuni[3*]

[1]*Department of Physics, National Institute of Technology Calicut, Calicut, Kerala, India*

[2]*Department of Mechanical Engineering, National Institute of Technology Calicut, Calicut, Kerala, India*

[3]*Department of Materials Science and Engineering, National Institute of Technology Calicut, Calicut, Kerala, India*

*Corresponding Author E-mail: aparnazagabathuni@nitc.ac.in

ABSTRACT

The oceans, covering over 70% of Earth's surface, present a significant opportunity for renewable energy through wave action. This study explores a clamp-based fixed-ended flexible beam designed for energy harvesting from sea waves, leveraging the dynamic response of flexible beams subjected to periodic wave forces to convert mechanical energy into electrical energy. A key innovation of this design is the central clamp-based mechanism, which is a distinctive feature of this study. In this setup, one end of the secondary frame connects to a floating tube that moves freely in the vertical direction, while the other end is securely clamped to the beam (Piezo Cell). This configuration fixes the beam at both ends, enabling it to undergo significant deflections when subjected to wave-induced forces via the clamp. The central clamp and rods act as axes, enhancing the beam's deformation and increasing the transmission of mechanical stress. This novel design improves the system's response to varying sea wave strengths, maximizing stress distribution across the beam and thereby enhancing its piezoelectric response. The flexible beam consists of three layers: a piezoelectric layer made of polyvinylidene fluoride (PVDF), with graphene serving as the top and bottom electrodes. Integrating PVDF with advanced conductive materials like graphene represents a promising approach to enhance energy harvesting from sea waves, ultimately improving the efficiency of renewable energy technologies. The dynamic behaviour of the beam is modelled using COMSOL Multiphysics, which simulates wave interactions with varying beam dimensions to predict the system's response. The results indicate that the energy harvesting capabilities of the flexible beam can vary significantly based on its dimensions. For instance, increasing the beam's length results in greater deflection under wave-induced loads, enhancing energy harvesting potential. However, excessive length may compromise structural stability. Conversely, a thicker beam typically exhibits reduced deflection due to increased stiffness, which may decrease energy harvesting efficiency. Additionally, changes in dimensions affect the beam's natural frequencies; longer beams tend to have lower frequencies, which can be beneficial for resonant energy harvesting. Furthermore, variations in geometry alter stress distributions and damping characteristics within the beam, impacting its durability and performance over time.

Keywords: Energy Harvester; Sea Waves; Clamped Beam; PVDF.

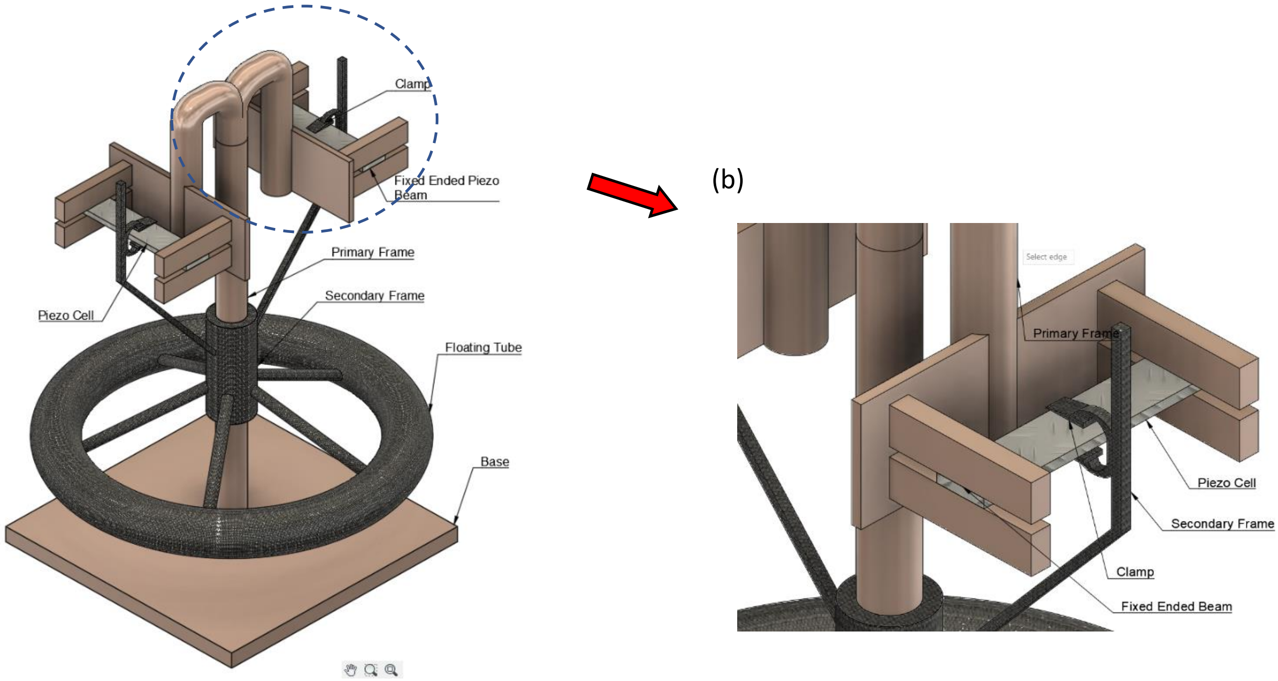

Figure 1: (a) Piezoelectric Sea Wave Energy Harvester, and (b) Central clamp-based mechanism

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Scalable Optofluidic Microreactors for Visible-light-driven Photocatalytic Overall Water Splitting: A Novel Approach Towards Commercialization

Ameer Suhail[1,*], D Pamu[1,2], Nageswara Rao Peela[1,3]

[1] *Centre for Nanotechnology, IIT Guwahati, Guwahati, Assam, India*

[2] *Department of Physics, IIT Guwahati, Guwahati, Assam, India*

[3] *Department of Chemical Engineering, IIT Guwahati, Guwahati, Assam, India*

*Corresponding Author E-mail: ameer@iitg.ac.in

ABSTRACT

This research presents an engineering framework for designing, fabricating, and implementing a high-performance scalable optofluidic microreactor for enhanced photocatalytic water splitting to generate hydrogen, incorporating a solar concentrator (fresnel lens) for both lab-scale and outdoor solar-driven water splitting. The microreactor fabrication utilizes photolithography-assisted wet chemical etching on commercial window glass sheets, with optimization experiments conducted for epoxy coating, laser engraving, and etching. A Z-scheme heterostructured photocatalyst system is developed, comprising Mo-doped $BiVO_4$ and g-C_3N_4 nanosheets, with added cocatalysts and TiO_2 nanoparticles as an electron mediator and film binder. The catalyst is immobilized on reactor walls by spray coating and characterized using various techniques. Performance evaluation includes assessing H_2 & O_2 evolution rates, a 20-hour stability test, and gas chromatography analysis. Scalability is demonstrated through a lab-scale unit with an A4 paper-sized fresnel lens and an outdoor solar-driven system featuring a larger optofluidic microreactor (11.5 in x 15 in) and a 1.1m x 1.1m solar concentrator. The research validates efficiency and scalability, contributing to global energy needs and sustainable energy transition, while providing insights into challenges and opportunities for large-scale implementation and informing future optimization strategies for industrial-scale photocatalytic hydrogen production facilities.

Keywords: Photocatalytic water splitting; Optofluidic microreactor; Hydrogen generation; Solar energy conversion; Z-scheme heterostructured catalyst.

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Impact of Corn Waste-Derived Biochar on Soil Properties and Plant Growth Parameters

Dharshini Jenifer A and Vaishakh Nair*

Department of Chemical Engineering, National Institute of Technology Karnataka Surathkal, India

*Corresponding Author E-mail: vaishakhnair@nitk.edu.in

ABSTRACT

India generates a substantial amount of agricultural waste annually, with estimates ranging from 516 million tonnes to 696.38 million tonnes. Corn along with other cereal crops contributes about 364.27 million tonnes of residues annually. A significant portion of crop waste, approximately 178 million tonnes, is burned annually due to a lack of sustainable management practices, hence this study focuses on using corn stover biomass which is a valuable source of organic matter that can be transformed into biochar through the pyrolysis process. The optimal production conditions for corn stover biochar were determined using the statistical method followed by the analysis of plant growth parameters and soil properties before and after the addition of biochar. It is found that biochar increases the soil nutrient content, water-holding capacity, and specific gravity of soil which subsequently leads to increased plant growth.

Keywords: Agricultural waste; Soil properties; Statistical methods; Plant growth; Pyrolysis.

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Development and Characterization of TPU-PLA Blends for Enhanced Shape Memory Performance for Biomedical Applications using SLA 3D Printing

Paritosh Tomar, P Sumanth, P Vishalini, Aparna Zagabathuni*

Department of Materials Science and Engineering, National Institute of Technology Calicut, Calicut, Kerala, India

*Corresponding Author E-mail: aparnazagabathuni@nitc.ac.in

ABSTRACT

The blend of thermoplastic polyurethane (TPU) and polylactic acid (PLA) has garnered significant attention in the field of biomedical applications due to favourable mechanical properties and biocompatibility. TPU is known for its excellent flexibility, durability, and strength, while PLA is recognized for its biodegradability and biocompatibility, making this combination particularly suitable for medical devices and tissue engineering. The ability to tailor the mechanical properties through composition adjustments enables the development of scaffolds that can mimic the mechanical behaviour of natural tissues, which is crucial for successful integration within the body. Stereolithography (SLA) 3D printing offers superior dimensional accuracy, the ability to print flexible materials, faster print speeds, and higher potential productivity compared to other additive manufacturing methods. This study focuses on the development and characterization of thermoplastic polyurethane (TPU) and polylactic acid (PLA) blends to achieve a fast shape memory effect using an SLA 3D printing process. The TPU-PLA blend was prepared in a different ratio (30:70, 50:50, 70:30) and the influence of printing parameters such as exposure time, layer thickness, and printing speed on the mechanical properties and shape memory capabilities have been identified. The morphology of the printed samples was analysed using scanning electron microscopy, confirming a compatible blend structure conductive to shape memory effect. The 30% TPU blend enhanced the tensile strength compared to pure PLA, but excessive TPU lead to decrease in strength due to phase separation. TPU's high elongation contributes to the overall ductility of the blend. Belding TPU with PLA improves impact resistance significantly making them more suitable for load bearing applications. This work not only highlights the potential of TPU-PLA blends for rapid prototyping applications but also provides critical insight into optimizing SLA parameters for enhanced shape memory performance.

Keywords: Polymeric Blend; Shape memory effect; Bio-mimicking; SLA 3D printing.

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Interface Optimization of Silicon Oxycarbide Ceramic-Coated Electrodes for Enhanced Electrochemical Performance

Samudrala Nagarani[1*], Jella Gangadhar [1], Chanchal Chakraborty[2], **Ravindran Sujith[1]**

[1]*Mechanical Engineering Department, Birla Institute of Technology and Science Pilani, Hyderabad Campus, 50078 India*

[2] *Chemistry Department, Birla Institute of Technology and Science Pilani, Hyderabad Campus,50078 India*

*Corresponding Author E-mail: p20220428@hyderabad.bits-pilani.ac.in

ABSTRACT

Amorphous silicon oxycarbide ceramics (Si-O-C) derived from Si-based polymeric precursors are promising for electrochemical applications, such as lithium-ion and sodium-ion batteries, due to their versatility and excellent chemical stability. However, achieving a smooth electrode-to-current collector interface remains a key challenge. Optimization of electrode interfaces is critical in order to enhance electrochemical performance in energy storage devices. This paper discusses the interface engineering on electrodes coated with silicon oxycarbide (Si-O-C) ceramic coatings, which plays an important role in contributing to enhanced electrochemical behavior. In this study, the interface properties of silicon oxycarbide ceramic-coated electrodes were evaluated using copper film and CNT buckypaper as current collectors. The effect of ceramic particle size on interface properties was also investigated, using ball milling particle sizes were reduced to 50 nm, 200 nm, and 600 nm. Contact angle measurements using the sessile drop test revealed improved wettability for the Si-O-C buckypaper system. The surface free energy, determined via the Owens-Wendt-Rabel-Kaelble method, was found to be 49.02 mN/m for CNT buckypaper and 37.98 mN/m for copper films. Scanning electron microscopy confirmed a smoother interface in the Si-O-C-coated buckypaper system. Additionally, electrical conductivity and cyclic voltammetry studies were performed on both systems.

Keywords: Batteries; Polymer derived ceramics; Surface free energy; Interface; Electro-chemical properties.

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Synthesis And Study of Plasmon-Enhanced Characteristics of Au@Ag@Polymer Bimetallic Core-Shell Nanoparticles for Energy and Environmental Applications

Thirumalesh B S*, Dr. Ramesh Asapu

[1]*Department of Chemical Engineering, Indian Institute of Technology Jodhpur, NH 62 Nagaur Road, Karwar, Jodhpur 342037, India*

*Corresponding Author Email: p22ch008@iitj.ac.in

ABSTRACT

Plasmonic metal nanoparticles have attracted researchers due to their unique LSPR characteristics which make them suitable for the applications like sensors for medical and pharma applications as well as energy and pollution control related applications in the form of photocatalysts. Among the plasmonic materials, gold and silver are extensively investigated because of their surface plasmon characteristics in the visible range. However, a fixed plasmon resonance for a given geometry of the gold and silver plasmonic nanoparticles have limited their applications as a photocatalytic material. Also, the stability issues with silver nanoparticle when compared to gold nanoparticle further limits its usability for commercial applications. On the other hand, the addition of second metal with varying composition could alter the frequency, quality factor, and decay pathways of the surface plasmon resonances of single metal nanoparticles, which allows the tuning of the absorption to scattering ratio and hence reaction selectivity of bimetallic plasmon nanoparticles such as core@shell type arrangement or metal alloy type combination. Also, the protective layer surrounding these metal nanoparticles could sufficiently provide stability to these bimetal plasmonic nanoparticles. Layer by layer synthesis of ultrathin insulating polymer coating surrounding the plasmonic metal nanoparticles have been extensively researched. This technique utilizes a simple procedure to create a thin protective shell of size ranging from 1.5-5 nm around the metal nanoparticles. The major property to investigate here is the effect of polymer coating on the local electric field enhancement of plasmonic metal nanoparticles when irradiated with light in the UV-Visible spectral region. In this study an insulating polymer coated plasmonic Au@Ag bimetallic core shell metal nanoparticles were synthesized and their experimental plasmon enhanced characteristics were analysed via Raman spectroscopy and were compared theoretically using the finite element method using COMSOL Multiphysics tool (V6.2). It was found that bare Au@Ag core- shell bimetallic nanoparticles showed enhanced electric field followed by 4 layered and for 8 layered bimetallic nanoparticles it was not that significant. XPS analysis was also performed to confirm the elements present in the polymer coated Au@Ag nanoparticles. These studies may be useful in utilizing bimetallic plasmonic core-shell nanoparticles for semiconductor photocatalysis were systems like Au@Ag/TiO_2 could be tested for its photocatalytic activities and further may be used for plasmon enhanced photocatalysis applications especially for energy and environmental challenges such as hydrogen generation and air pollution control strategies.

Keywords: Bimetallic gold @silver NPs; Plasmon shift; Raman spectra; Near- field enhancement; COMSOL.

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Wet Chemical Synthesis and Characterization of Ethylene Glycol Encapsulated Manganese Oxide Nanorods

Biswajith S[1], A Martin Joseph[2,*]

[1]*Department of Materials science and engineering, National Institute of Technology Calicut, NIT Campus (P.O.), Kozhikode 673601, Kerala, India.*

[2]*Achariya Siksha Mandir, Villianur, Puducherry –605 110, India.*

*Corresponding Author E-mail: a.martinjoe@gmail.com

ABSTRACT

In recent years, optimized architectural manipulation of transition metal oxide with well-defined surface morphology and tuneable dimension has been the centre of intensive research because of their potential excellence in photonics, catalysis, magnetic applications and in mechanical applications. In the present work, Manganese oxide nanorods were prepared by reducing $KMnO_4$ with $Na_2S_2O_3.5H_2O$ by encapsulating with ethylene glycol. The structural, functional, morphological and chemical composition of the nanorods were investigated by X-Ray Diffractometer (XRD), Fourier Transform Infrared Spectrometer (FTIR), High Resolution Scanning Electron Microscope (HR-SEM) and Energy Dispersive X-Ray Spectrometry (EDX). From XRD analysis the 2θ peaks around 28.8°, 37.5° and 49.86° indicated the high crystalline nature of the product. FTIR confirmed the contribution of the organic ligand in surface passivation. HR-SEM image revealed the formation of MnO_2 nanorods sizing to an average of 30 x 200 nm. EDX confirmed the presence of Mn and O in the material. Absorption behavioural study done through UV–visible spectrophotometer identified an indirect band gap of 1.37 eV as acquired by Taucplot.

Keywords: Nanorods; Chemical synthesis; Manganese oxide.

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Photocatalytic Dye Degradation of Mixed Dyes Using Zinc Oxide Nanoparticles

C Shalini[1], K K Nagaraja[2], S Pramodini[1, *]

[1]*Department of Physics, REVA University, Kattigenahalli, Yelahanka, Bengaluru-560064, India.*

[2]*Department of Physics, Manipal Institute of Technology, Manipal, Manipal Academy of Higher Education, Manipal-576104, India.*

*Corresponding author: somynraj@gmail.com

ABSTRACT

The present work focuses on enhancing the photocatalytic degradation efficiency of Rhodamine B (RhB) in the presence of Acid blue (AB 25) using Zinc Oxide (ZnO) nanoparticles synthesized using Sol-Gel method. The photocatalytic degradation of single and binary dye was studied under UV-light source for 2 hours. AB 25 demonstrated 87.43 % (for 200 μM) degradation at the rate of 0.0133 min^{-1} with 1 g/L catalyst loading. Similarly, RhB (for 50 μM) dye exhibited 62.66 % degradation at the rate of 0.0064 min^{-1}. Whereas, RhB (50 μM) displayed better degradation of 94.18 % at the rate of 0.0204 min^{-1} after the addition of AB 25 (50 μM) dye. The enhancement in the degradation efficiency may be attributed to the shift in the emission wavelength and decrease in the intensity of the peak with increase in the AB 25 concentration in the binary solution and the same was confirmed with Photoluminescence (PL) analysis. When compared with the previously published literature reports, we have achieved better degradation efficiency of 94.18 % for binary dyes.

Keywords: Photocatalytic degradation; Binary dye; UV light.

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Design and Fabrication of Low-Impact Resistant Waterproof Car Cover in mitigating of Flood Damage

P Vigneshkumar, Nijo Prasad, V Sakthivel, M V Prithviraj*

Mechanical Engineering, Kamaraj College of Engineering and Technology (Autonomous), S.P.G.Chidambara Nadar – C. Nagammal Campus, S.P.G.C. Nagar, K. Vellakulam - 625701, Virudhunagar, India.

*Corresponding Author E-mail: m.v.prithiviraj@gmail.com

ABSTRACT

Floods are a recurring natural disaster in Chennai, causing extensive damage to vehicles parked in low-lying areas. This research focuses on the design and fabrication of a low-impact resistant, waterproof car cover using low-density polyethylene (LDPE) to mitigate the effects of flooding. The goal is to develop a cost-effective solution that can protect vehicles from flood damage by preventing water infiltration and providing structural protection against low-impact forces. LDPE was selected for its favourable properties, such as flexibility, durability, and water resistance, making it suitable for flood-related applications. The car cover is designed to envelop the vehicle fully, creating a waterproof barrier that protects key components, including the engine, electrical systems, and interiors. A key challenge addressed in the design was ensuring the cover remained lightweight and easy to install while providing adequate protection from floating debris, which can cause minor but costly damage during flooding. The fabrication process involved heat-sealing LDPE sheets to form an impermeable layer, with reinforced seams to ensure durability under pressure. Testing involved exposing the cover to controlled water immersion and simulated low-impact forces to evaluate its performance under conditions mimicking flood scenarios in Chennai. The results demonstrated the car cover's ability to prevent water ingress and withstand minor impacts from floating debris, thus offering significant protection against flood-related vehicle damage. This research provides a practical and scalable solution for vehicle owners in flood-prone regions like Chennai. The low-cost, easy-to-manufacture LDPE car cover presents a viable approach to minimizing the financial burden associated with vehicle repair after floods, contributing to better preparedness and resilience against natural disasters.

Keywords: Waterproof protection; Flood Resilience; Vehicle Preservation; Seamless Coverage; Weather Durability.

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Theoretical Insights into (Opto) Electronic Tuning of Naphthalene Diimide-Naphthodithiophene (NDI-NDT) Copolymers for Organic Electronics

Swathi Suneesh, Sushri Soumya Jena, Sarbani Ghosh, and Mohit Garg*

Department of Chemical Engineering, Birla Institute of Technology and Science (BITS),

Pilani Campus, Vidya Vihar, Pilani, 333031, Rajasthan, India

*Corresponding Author E-mail: mohit.garg@pilani.bits-pilani.ac.in

ABSTRACT

Naphthalene diimide (NDI)-based donor-acceptor (D-A) copolymers have attracted considerable interest within the realm of organic electronics, specifically in organic field-effect transistors (OFETs) and organic solar cells (OSCs), owing to their tunable (opto) electronic characteristics. While various donor units, such as thiophene and selenophene, are widely studied in combination with NDI, there is a growing interest in employing novel donor moieties to achieve balanced n-type and p-type behaviour. Naphthodithiophene (NDT) is a promising donor moiety in organic electronics due to its ability to enhance optical absorption and reduce the band gap when combined with suitable acceptor units. The extended π-conjugation and planar conformation of NDT facilitate enhanced charge transport and improved (opto) electronic properties, rendering it a viable candidate for the attainment of balanced n-type and p-type characteristics in D-A frameworks. However, the use of NDT in combination with NDI has been relatively unexplored in both experimental and theoretical studies. We present a comprehensive theoretical study on the (opto) electronic properties of NDI-NDT copolymers using density functional theory (DFT) and time-dependent DFT (TD-DFT) across various redox states up to 200%. Our results demonstrate a significant band gap reduction to 1.55eV upon incorporation of NDT. Additionally, we observe a pronounced red shift in the optical absorption spectrum during doping, extending from 300 nm to 900 nm. This tunability of the electronic and optical properties highlights the potential of NDI-NDT copolymers for high-performance OFET and OSC applications, offering balanced n-type and p-type behaviour essential for efficient charge transport.

Keywords: Naphthalene diimide; Naphthodithiophene; Organic field-effect transistors; Organic solar cells.

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High-Performance Hydrogen Sensing Using Zr co-doped ATO Thin Films

Sneha C* and Soney Varghese

Department of Materials Science and Engineering, National Institute of Technology, Calicut, India

*Corresponding Author E-mail: sneha_p210092mt@nitc.ac.in

ABSTRACT

This study focused on developing hydrogen gas sensors by fabricating Zr co-doped ATO thin films on SiO_2/Si substrates using the RF magnetron sputtering technique, conducted at a substrate temperature of 300°C. The films were characterized by X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Energy-Dispersive X-ray Spectroscopy (EDS), current-voltage (I-V) analysis, temperature-dependent wettability studies, and gas sensing measurements. SEM analysis revealed a granular morphology with a porous structure, enhancing the gas-sensing capabilities of thin film. EDS confirmed the elemental composition, with Zr content increasing as the DC power of magnetron sputtering was raised from 50 to 80W. The co-doped films exhibited hydrophilic behaviour, with contact angles decreasing from 89° to 59°, further improving moisture evaporation at higher temperatures, which reduced interference in gas sensing. Electrical measurements indicated semiconductive behaviour, with increased conductivity due to Zr doping. Additionally, the activation energy was calculated and found to decrease with increasing Zr deposition power. Hydrogen gas sensing tests were performed for a heavily doped Zr, showing a maximum detection limit of 0.5ppm at 150°C, with response and recovery times of 14 seconds and 10 seconds, respectively. The film exhibited a sensitivity of 4%, demonstrating its potential for efficient hydrogen detection.

Keywords: H_2 gas detection; RF sputtering; Zr co-doping; ATO thin films.

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Efficient Synthesis of Carbon Nanospheres from Polystyrene using Microwave-Initiated Biochar Based Bimetal-Catalytic Method

Sreeja P, Vineesh Ravi*
Department of chemical engineering, National Institute of Technology, Calicut, Kerala
*Corresponding author E-mail: vineeshravi@nitc.ac.in

ABSTRACT

This research looks into the huge potential of biochar-supported bimetallic catalysts for synthesising carbon nanomaterials using a microwave synthesizer from polystyrene and Low-density polyethylene (LDPE) at 600W, 90 seconds and 900 W at 30 minutes respectively, which is a quick and easy method that uses little energy. We used bimetallic catalysts with different composition of active metals Fe, Co, Ni in the ratio 1:3,3:1 and 1:1. The synthesised catalysts were analysed using different techniques. These methods included CHN analysis, XRD, SEM, HRTEM, and Raman spectroscopy. Biochar has more carbon than raw wood sawdust (48.23%), according to a CHN study. This makes biochar a great support material for bimetallic catalysts. The Fe: Co (1:3)/Mo/biochar catalyst had the best surface area, pore diameter, and pore volume of all the ones that were tried. It also produced the most CNS (78.5%). XRD analysis showed the presence of metal oxides and spinel structures, which means that the catalyst formation went well. Carbon nanospheres with sizes ranging from 16 to 300 nm were found using SEM and HRTEM. HRTEM confirmed that the nanospheres were not solid but rather amorphous. Raman spectroscopy showed that Fe: Co (1:3)/Mo/biochar had the lowest Id/Ig number (0.82), which means it had fewer defects and more graphitization than the other catalysts. The study shows that cobalt is very important for making the CNS, especially when it is present in higher amounts than iron. It also shows that iron and cobalt work together to make the CNS more plentiful and better quality. In conclusion, this study shows that biochar-supported bimetallic catalysts work well in microwave synthesis. This gives us important information for improving the production of carbon nanomaterials.

Keywords: Carbon nanospheres (CNS); Polystyrene; Biochar; Microwave synthesiser; Bimetallic catalyst.

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Improving Surface Wettability of $WO_3.0.33H_2O$ Nanostructures for HER Catalysis

Angelin Abraham, M Junaid Bushiri*

Department of Physics, Cochin University of Science and Technology, Cochin, India

*Corresponding Author Email : junaidbushiri@cusat.ac.in

ABSTRACT

Tungsten oxide (WO_3) is an attractive metal oxide electrocatalyst that is widely exploited for its versatile intrinsic properties. Understanding the surface properties of the WO_3 electrocatalyst, such as surface wettability, will give additional insights into the mechanism of electrochemical hydrogen evolution reactions (HER). Hydrophilic electrocatalysts can facilitate faster electrode-electrolyte contact and, thereby, better HER reactivity. This work explores the surface wettability of $WO_3.0.33H_2O$ nanostructures regulated via a hydrothermal process. The morphology and structural composition are experimentally confirmed using FE-SEM, XRD, FTIR, and Raman analyses. The water contact angle measurements of synthesised samples revealed enhanced wettability with a contact angle of 15° at a hydrothermal synthesis temperature of 200°C. The improved wettability and the presence of lattice water in the $WO_3.0.33H_2O$ sample can be further utilised for HER catalysis.

Keywords: Tungsten oxide; Hydrothermal Synthesis; Hydrophilic Surface; HER catalysts.

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Design and evaluation of vanadium pentoxide coated smart windows for passive radiative cooling applications

P Uma Sathyakam[1,*], Dhruv gupta, Rishabh Bhaumik, R Vijayaraghavan[2]

[1]*School of Electrical Engineering, Vellore Institute of Technology, Vellore, India*

[2]*School of Advanced Sciences, Vellore Institute of Technology, Vellore, India*

*Corresponding Author E-mail: umasathyakam.p@vit.ac.in

ABSTRACT

Passive radiative cooling based smart windows are emerging as a potential solution for reducing energy needs of buildings, both homes and offices alike. While lot of research has occurred in this regard, vanadium oxide-based materials are studied very recently. We carry out a finite element method-based simulation study to understand the behaviour of using Vanadium pentoxide (V_2O_5) as a coating on glass windows. The proposed design can help in saving energy by emitting cooler rays inside the building when direct sun rays fall on the coated glass surface, thereby reducing internal room temperatures. It is also a solution to global warming as the emissions from ACs will reduce due to lower inside temperature of the building thereby reducing demand on power usage. We found that the ambient temperature (T_{amb}) inside buildings can be reduced by up to 8 °C when the outer temperature is 40°C. Also, the surface radiosity of V_2O_5 windows is twice that of glass windows and increased with outer temperature. Lastly, we compare the performance of V_2O_5 with that of VO_2 and find that they have similar characteristics of radiant exitance, surface radiosity and surface emissivity of long wave infrared (LWIR) rays thus making V_2O_5 as a possible candidate for passive radiative cooling (PRC) which is low cost and affordable than VO_2.

Keywords: Passive radiative cooling; Smart windows; Vanadium pentoxide; Buildings; Cooling windows.

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Synthesis and Characterisation of Bio-Nanocomposite Coated Urea Nanofertilizers

Praseetha P Nair* and Feba Mohan M

Department of Chemical Engineering, Government Engineering College, Thrissur-680009, Kerala, India.

*Corresponding author E-mail: praseethajayan@gmail.com

ABSTRACT

A bio-nanocomposite of carboxymethyl cellulose (CMC), nano-hydroxyapatite (nano-HA), nano-clay, and urea was synthesized using two different methods: dry ball milling in a planetary ball mill and solvent casting. Urea release from these composites was evaluated via water immersion experiment. Comparative analysis revealed that the solvent-casted nanocomposites exhibit significant reduction in urea release than the dry-milled composites, prompting the selection of solvent casting for subsequent synthesis. To improve the field applicability of urea, the bio-nanocomposite mixture was coated onto urea particles. A comparison of coated and uncoated urea samples demonstrated that the coating significantly prolonged urea release. While uncoated samples released all nutrients within two days, the coated samples sustained release for five days. These findings suggest the potential of this bio-nanocomposite for controlled nutrient delivery in agricultural applications.

Keywords: Bio-nanocomposites; Planetary ball milling; Solvent casting; Urea nanofertilizers.

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Pressure Resistant Multifaceted 3D Bioprinted Biopolymer Scaffold for Lung Epithelial Cells: A Mechanotransduction Study

Abey Joseph [1], Athira S Vijayan[2], Nigina Gopinath[1], Baiju G Nair[1,*]

[1]*Department of Bioscience and Engineering, National Institute of Technology Calicut, Kozhikode, India*

[2] *Department of Materials Science and Engineering, National Institute of Technology Calicut, Kozhikode, India*

*Corresponding Author E-mail: bgnair@nitc.ac.in

ABSTRACT

The extracellular environment (ECE) is of predominant importance to a cell's life. A few extracellular cues that mold cells include chemical components (nutrients, growth factors, messengers, hormones, and enzymes), temperature, pressure, mechanical strength of the adhesion matrix, and light. Hence, to study a group of cells outside the living body, a similar ECE is crucial to mimic an in vivo cellular response. Through this work, we are developing a system that mimics the cellular environment of mammalian lungs. There are more than 25 commonly known diseases affecting human lungs, most of which have molecular connections with ECE; however, most of the research involving these diseases is performed on monolayer culture without the apt environment. This study addresses this issue. The lobes and alveoli are two significant parts of the lungs that are difficult to mimic in vitro. This is because of the varying air pressure and perfusion of blood through the capillaries. To better mimic in vivo systems, 3D cell culture was used to grow the cells. 3D bioprinting using an indigenously developed bioink was used to fabricate a tailorable scaffold for various applications. This scaffold provides the requisite cellular environment that mimics the extracellular matrix. The microporous scaffold, supported by a stainless-steel mesh enclosed in a casing, provides a barrier to separate the air and liquid phases. The scaffold was characterized to obtain the tensile strength, Young's modulus, elasticity, and compressive strength, which proved that the developed scaffold matched the in vivo system. MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) assay and cell counting kit – 8 (CCK-8) were performed to confirm biocompatibility. After subjecting the bioprinted cells to varying air pressures (-20 to +20 mmHg), their morphology was observed through rhodamine-DAPI (cytoskeletal staining) and Calcein-AM/PI (live dead) staining. SEM was used to observe the morphology of the cells in detail. After exposure to varying pressures, cells were observed for cell migration, which is indicative of cell health. Although this study deals with cell behavior, the system can be utilized for the development of lung disease models, drug testing, toxicity studies, and molecular pathway elucidation.

Keywords: Extracellular environment; Cell behaviour; 3D bioprinting; Biopolymer; Microporous scaffold.

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Uptake and Accumulation of Micro/Nanoplastics in Terrestrial Plants: Insights from Carbon Dot-Embedded Polystyrene Interactions with Legumes

Nigina Gopinath[1], Abey Joseph[1], Athira S Vijayan[2], Sajith V[2], Baiju G Nair[1,*]

[1]*Department of Bioscience and Engineering, National Institute of Technology Calicut, Kerala, India*

[2]*Department of Material Science and Engineering, National Institute of Technology Calicut, Kerala, India*

*Corresponding Author Email: bgnair@nitc.ac.in

ABSTRACT

Microplastics (MPs) and nanoplastics (NPs) are pervasive environmental pollutants, raising concerns about their impact on terrestrial ecosystems, particularly agricultural crops. This study investigates the uptake and translocation of fluorescent carbon dot embedded polystyrene (CDPS) as a model for studying microplastic behaviour in leguminous plants, *Vigna radiata* (Green Gram) and *Vigna angularis* (Adzuki Bean). CDPS particles were synthesized via mini-emulsion polymerization, using hydrophobic carbon dots derived from candle soot. Characterization of CDPS was performed through UV–Vis spectroscopy, zeta potential analysis, and fluorescence microscopy. Plant exposure studies were conducted in hydroponic systems with varying concentrations of CDPS (2–100% v/v). Fluorescence microscopy and scanning electron microscopy (SEM) were used to trace the accumulation and movement of CDPS in plant tissues. Results revealed that CDPS particles translocated from roots to shoots through apoplastic pathways, accumulating in the vascular and cortical regions. Fluorescence was observed at concentrations above 6% v/v, confirming CDPS localization in the xylem. This study demonstrates the utility of CDPS as a fluorescent marker for tracing plastic particles in edible plants, with significant implications for food safety and environmental health. The findings highlight the potential risks of plastic contamination in agriculture, underscoring the need for further research on plastic translocation in crop plants.

Keywords: Micro-nanoplastics; Fluorescent carbon dots; Translocation; Leguminous plants; Environmental health.

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Wire-bonded Micro Heat Pipes: A Computational Study with Different Working Fluids

R L Rag[1], C B Sobhan[2], Rupesh S[3,*]

[1]*Younus College of Engineering and Technology, Kollam, Kerala 691010, India*

[2]*National Institute of Technology, Calicut, Kerala 673601, India*

[3]*PES College of Engineering, Mandya, Karnataka 571401, India,*

*Corresponding Author E-mail: mailtorupeshs@gmail.com

ABSTRACT

Efficient energy utilization is inevitable for sustainable development through establishing energy security and reduced environmental impacts. Energy utilization in electronic devices can be optimized by maintaining proper heat dissipation as operating temperature has a crucial role in the performance of electronic components. Heat dissipation from electronic devices becomes challenging when the components have small size and high packing density. Micro heat pipes are widely applied in heat dissipation systems, particularly in electronics. Arrays of wire-bonded micro heat pipes are relatively simple to design. As the working fluid plays a crucial role on the performance of micro heat pipes, a computational study was conducted to quantify the influence of geometrical parameters on the performance characteristics of wire-bonded micro heat pipes using different working fluids. The length of the condenser section is the geometrical parameter considered in the analysis. A copper heat pipe with water, acetone, and methanol as the working fluids was considered for the analysis. The longitudinal variations in the cross-sectional areas of the liquid and vapor and the temperature-dependent thermo-physical properties of the working fluids were used in the analysis. The temperature distributions obtained by solving the governing equations using a finite difference scheme were used for evaluating the performance of the device, and the effective thermal conductivity was used as the performance index. Among the wire bonded micro heat pipes considered, those with acetone and water show maximum performance with effective thermal conductivity values 181 kW/mK and 174 kW/mK for an evaporator heat influx of 2.0 W/cm^2. But when methanol is the working fluid, the maximum effective thermal conductivity value is only 68 kW/mK for an evaporator heat influx of 0.75 W/cm^2. The results were verified experimentally, and their applicability was evaluated for the temperature range appropriate for the material–fluid combination used.

Keywords: Wire-bonded Micro heat pipes; Thermo-physical properties; Effective thermal conductivity; Geometrical parameters; Operating parameters.

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Development of PLA-PCL based Bio-Nanocomposite Implant Material Enhanced with Hydroxyapatite

Litha T T, Praseetha P Nair*

Department of Chemical Engineering, Govt. Engineering College,

Thrissur, 680009, Kerala, India

*Corresponding Author E-mail: praseetha@gectcr.ac.in

ABSTRACT

Polylactic acid offers a promising alternative to conventional plastics, offering biodegradability, renewability, and versatility. Indeed, blending PLA with other polymers and reinforcing it with nanofillers are common strategies employed by researchers to enhance its biomechanical properties. PCL, a biodegradable polymer, is compatible with PLA, making it an ideal candidate for blending. This compatibility enables the enhancement of PLA's properties through blending. Both PLA and PCL are regarded as biomedical materials by the Food and Drug Administration, USA, due to their biocompatibility. Both inorganic and carbon-based nanofillers were incorporated in the polymer nanocomposite preparation. The inorganic filler, such as Montmorillonite nanoclay (MMT), was integrated into the polymer nanocomposite at concentrations varying from 1 to 4 wt%, while graphene oxide (GO) and reduced graphene oxide (rGO) were utilized as carbon-based nanofillers within the composite, ranging from 0.02 to 0.1 wt%. To create superior materials, blends of PLA and PCL reinforced by HA with varying weight percentages of 10 to 45 wt% are also taken into consideration. The biological properties such as biodegradation, porosity, and swelling of polymeric bio-nano composites were then investigated. Here, in the present work, it is attempted to synthesize polymer bio-nano composites suitable for biomedical implants based on PLA/PCL blend reinforced with HA and GO.

Keywords: Polylactic acid (PLA); poly (Ɛ-caprolactone); Graphene Derivatives; Hydroxyapatite (HA); Solvent casting.

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Corrosion Inhibition of EDTA for 304 L Steel in 1M HCl

Hafin Shan P K*, Adeeb Adam M V, Ashmil Mohammed, Aabid Abdul Latheef K P, M D Bindu

Department of Mechanical Engineering, Government Engineering College, Thrissur-680009, Kerala, India

*Corresponding Author E-mail: shanhafin7592@gmail.com

ABSTRACT

In process industries hydrochloric acid is stored and transported in 304 L tanks and pipes at room temperatures. These tanks and pipes undergo severe corrosion overtime causing heavy losses to the industries. Any method to retard this corrosion and increase their life span is of prime concern. This paper investigates the corrosion inhibition mechanism of ethylenediaminetetraacetic acid (EDTA) on austenitic stainless steel 304 L in HCl solution. The corrosion rate of SS 304 L was determined as 45.6 mpy by the gravimetric method. The experiments were repeated by adding three different concentrations of EDTA to the HCl solution viz 0.2g, 0.4g and 0.6g. The corrosion rate was 7.76, 5.63 and 6.03 mpy and the inhibition efficiency was 82.98 %, 87.65%, and 86.77 % with EDTA concentrations 0.2g, 0.4g and 0.6g respectively. The results indicate addition of 0.4g EDTA in HCl solution increases the inhibition efficiency and reduces rate of corrosion.

Keywords: Ethylenediaminetetraacetic acid (EDTA); Stainless Steel 304 L; Corrosion; HCl; Inhibition efficiency.

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Investigation on Structure Stability and CO_2 Adsorption Over Single Atom Catalyst Doped N-Defected Graphene: DFT and MD Studies

Kavipriya T, Premkumar S*

Department of Physics, Vellore Institute of Technology – Vellore campus, Tiruvalam Rd, Katpadi, Vellore, India

*Corresponding Author E-mail: premkumar.s@vit.ac.in

ABSTRACT

Single atom catalyst (SAC) supported on carbon-based materials shows immense activity towards CO_2 capture. Graphene with defects and heteroatoms doping helps to increase the CO_2 adsorption by providing more active sites to interact with CO_2 molecule. Significant research works have been carried out to study the CO_2 adsorption nature of nitrogen doped defected graphene (NDDG). The NDDG with graphitic, pyridinic and pyrrolic frameworks have not been explored well. Moreover, the SAC doped NDDG with two pyrrolic-N, two pyridinic-N, and one graphitic-N atoms located in the edges of the defected graphene has not been modelled and the CO_2 adsorption characteristic of the unique SAC doped NDDG is not yet explored. In this work, a systematic investigation was conducted using density functional theory (DFT) to analyse the structural and electronic properties of NDDG system with and without different SAC transition metals (TM) such as copper, nickel, iron and zinc. We reported the thermal stability of the pristine NDDG and SAC doped NDDG by Ab Initio molecular dynamic (AIMD) at room temperature (300K) with the aid of on-fly machine learning. The formation energy of the pristine NDDG and TM-SAC doped NDDG was calculated. The formation energy value of the pristine NDDG is -2.18 eV/atom. The calculated formation energy value of TM-SAC doped NDDG is ordered as Fe= -2.19 eV/atom > NDDG= -2.18 eV/atom > Ni= -2.17 eV/atom > Zn= -2.16 eV/atom > Cu= -2.16 eV/atom. The feasible CO_2 adsorption sites are predicted by analysing CO_2 adsorption energy in various adsorption sites of pristine and TM-SAC doped NDDG by placing the CO_2 on top of the system in a parallel or perpendicular position. The results revealed that the CO_2 placed in the parallel position on the TM-SAC doped NDDG has higher CO_2 adsorption capacity. The study shows that the iron (Fe)-SAC doped NDDG has good stability (-2.19 eV/atom) and higher CO_2 adsorption (-115.66meV/atom) activity among the materials considered.

Keywords: CO_2 adsorption; DFT; AIMD; Nitrogen doped defected graphene; Single atom catalyst.

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Low-Temperature Solvothermal Growth of Co_xS_y Nanospheres on Conducting Substrates as Efficient Electrodes for Hydrogen Evolution Reaction

Nabeel N Abu[1], Amal Benny[2], Aswathi Ganesan[1*]

[1]*Dept. of Physics, National Institute of Technology Calicut, Kozhikode, Kerala, India*

*Corresponding Author Email: nabeel.na.1996@gmail.com

ABSTRACT

Electrochemical water splitting is widely regarded as a sustainable method for green hydrogen production. An energy-efficient and cost-effective production of hydrogen through hydrogen evolution reaction (HER) requires highly active and low-cost alternatives to traditional noble metal-based catalysts such as platinum. Recently, cobalt sulfide materials like CoS_2, Co_3S_4, and Co_9S_8 garnered particular attention for electrocatalytic applications owing to their excellent metallic conductivity, good intrinsic activity, and earth abundance. Despite the progress in the development of efficient and non-noble metal-based electrocatalysts, their performance still falls behind platinum in terms of HER activity and stability. Furthermore, many of the existing synthesis methods are suitable for laboratories, require expensive synthesis facilities, and are difficult to scale up to the industrial level due to the complexity of the methods involved. In this work, we discuss a feasible, one-step solvothermal synthesis method to grow different sizes of cobalt sulfide (Co_xS_y) nanospheres made up of Co_3S_4 and Co_9S_8 on CC, which can be directly employed as a self-standing working electrode for catalyzing HER, without any use of polymer binders. The current synthesis method is facile and economical, requires less time, and can be processed at a very low temperature (80 °C), compared to many other previous reports on solvothermal methods. In addition, we studied the influence of utilizing various cobalt precursors during the solvothermal synthesis process and their effects on the morphological and electrocatalytic performance of the resulting Co_xS_y nanospheres. The morphology and fine structure of the synthesized samples were investigated using scanning electron microscopy, field emission scanning electron microscopy, and transmission electron microscopy. The structural and crystallographic information was obtained from Raman and X-ray diffraction spectrums of the sample. The chemical composition of the samples was analyzed using energy dispersive X-ray spectroscopy, and X-ray photoelectron spectroscopy. Electrocatalytic measurements revealed that incorporating multiple cobalt precursors during the synthesis is shown to have a positive influence on their HER electrocatalytic performance due to the changes in the particle size distribution and the number density on CC. The as-synthesized electrocatalyst materials (Co_xS_y/CC) showed good catalytic performance with reliable stability for HER in both acidic (0.5 M H_2SO_4) and alkaline media (1 M KOH), with overpotential values of 143 and 313 mV, respectively, for a current density of 10 mA/cm^2. Moreover, this synthesis method is a general procedure that can be potentially extended to other metal sulfides and for the production of efficient metal sulfide-based electrocatalysts in an effortless and feasible manner.

Keywords: Electrocatalysis; Hydrogen evolution reaction; Solvothermal reaction; Co_9S_8; Co_3S_4.

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Upcycling Waste Expanded Polystyrene for Sustainable Wood Plastic Composite: Mechanical and Water Absorption Properties

Bijo Abraham Jacob, Sudhanshu Nartam*, Ummen Sabu, Arun S, Jinu Paul, S Budhe

Department of Mechanical Engineering, National Institute of Technology (NIT) Calicut, NIT Campus P.O., Kozhikode, Kerala, India 673601

*Corresponding Author Email: sudhanshu_p210084me@nitc.ac.in

ABSTRACT

Still, expanded polystyrene (also called Thermocol) is widely used due to its shock-absorbing and insulation properties in many sectors. However, it poses serious environmental challenges, as it is not easily degradable. The main objective of this study is to convert expanded polystyrene (EPS) waste into eco-friendly adhesives and use them to produce wood-plastic composites (WPC). We optimized a mixed solvent of acetone and ethyl acetate to dissolve expanded polystyrene (EPS) waste, for high bonding strength and uniform dispersion for reinforcement. WPCs were produced by combining bamboo wood with an adhesive derived from EPS waste, based on a weight percentage in grams using the compression moulding method. Three different wood-to-adhesive ratios—50:50, 40:60, and 60:40—were selected for producing the WPCs. For reinforcement, a blend of bamboo pulp and fiber was used in a consistent 70:30 ratio across all samples. Mechanical, water absorption and thermal stability tests were conducted on all prepared WPC combinations to evaluate their performance. Modulus of rupture (MOR), modulus of elasticity (MOE), screw holding strength, and dimensional stability, measured as thickness swelling and water absorption were some of the key properties that were assessed. These tests determine the suitability of WPCs produced from waste materials. Results indicate that the mechanical properties of the composites vary with the wood-to-adhesive weight ratio. It was found that the WPCs produced from a 50:50 ratio of wood and adhesive have a higher MOR of approximately 21.42 N/mm^2 and MOE of 30,227 N/mm^2, which is equivalent to other WPCs made from a thermoplastic binder. Waste is a substantial global issue that urgently needs addressing to use resources and energy more efficiently, particularly as the packaging industry generates large amounts of thermocol waste each year, making recycling essential for sustainability. Addressing waste not only involves managing disposal but also creating valuable products from it, which can significantly reduce the accumulation of solid waste. Moreover, recycling and reusing waste EPS contributes to a greener and cleaner environment.

Keywords: Thermocol waste; Wood-plastic composite; Recycling; Sustainability; Composite Panel.

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Injectable PEGDA/HA Nanocomposite for Bone Regeneration with Osteoconductive Support

Abhijith M[1], Ashok Pannayamthatta[1], Varun Raghuveeran[1], Ashna Gauthaman[1,*], VP Muhammad Rabeeh[2]

[1]*Aster Research Foundation, Naseera Nagar, Wayanad, 673577, India*
[2]*Dr.Moopen's iNEST, Dr. Moopen's Medical College, Wayanad, 673577, India*

*Corresponding Author E-mail: ashna.gauthaman@drmoopensmc.ac.in.

ABSTRACT

Development of injectable, in situ curing biomaterials is a promising strategy for minimally invasive bone regeneration. This study presents the fabrication and comprehensive evaluation of a polyethylene glycol diacrylate/Hydroxyapatite (PEGDA/HA) nanocomposite, a potential candidate engineered injectable application in treatment of bone defects. The composite leverages osteoconductive properties of hydroxyapatite (HA) and tunable mechanical properties of PEGDA to support bone regeneration while conforming to irregular defect geometries. The PEGDA/HA nanocomposite were prepared though chemical curing of PEGDA incorporated HA nanoparticles, enabling *in situ* gelation. The structural characterization and investigation of filler-matrix interaction were systematically performed using FTIR spectroscopy and XRD analysis. Morphological characterization was conducted using field emission scanning electron microscopy (FESEM) to assess the surface structure and nanocomposite architecture. *In vitro* evaluation demonstrated favourable mechanical properties, with the composite exhibiting a high swelling capacity while preserving structural integrity and displaying controlled degradation rates, critical for its application in bone defect repair. Additionally, the osteoconductive behaviour of the material was validated through the differentiation of Mesenchymal Stem cells (MSCs) encapsulated in the hydrogel matrix, as indicated by enhanced alkaline phosphatase activity and calcium mineralization. These results demonstrate that the injectable PEGDA/HA composite provides an effective, minimally invasive platform for bone defect repair, offering osteoconductive support and mechanical stability while promoting bone tissue regeneration. This material holds significant potential for clinical applications in orthopaedic, craniofacial and spinal surgeries, where precise, customizable bone regeneration is critical.

Keywords: Hydroxyapatite; Polyethylene glycol diacrylate; Biomaterial, Mesenchymal Stem cells; Bone graft.

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Optimizing CNT Synthesis: Gaseous and Liquid Chemical Vapor Deposition Methods

K Raji[1], Ram Manohar Yadav,[2] Shijo Thomas[3], C B Sobhan[3] and P M Ajayan[4]

[1]*Department of Science and Engineering, Monash College, Monash University, Melbourne, Victoria 3008, Australia*

[2]*Department of Physics, Faculty of Science, University of Allahabad, Prayagraj, Uttar Pradesh, 211002, India*

[3] *Department of Materials Science and Engineering, National Institute of Technology, Calicut 673 601, India,*

[4]*Department of Mechanical Engineering & NanoEngineering, Rice University, Houston, Texas 77005, United States.*

*Corresponding Author E-mail: csobhan@nitc.ac.in

ABSTRACT

Chemical Vapor Deposition (CVD) has been demonstrated as one of the most promising methods for synthesizing carbon nanotubes (CNTs). The study presented here explores the effectiveness of CVD using two gaseous (acetylene and ethylene) and a liquid (xylene) precursor, with a focus on understanding the impact of critical process parameters such as furnace temperature, gas flow rates, and catalyst characteristics on the structural properties and purity of the CNTs. In the acetylene CVD process, iron oxide-coated ceramic substrates were heated in a tubular furnace to initiate CNT growth through acetylene decomposition. A similar approach was adopted for ethylene CVD, utilizing iron-coated silicon substrates. The liquid CVD method employed a ferrocene-xylene solution, where ferrocene decomposed to supply the iron catalyst essential for CNT formation. Characterization techniques, including Raman Spectroscopy, Scanning Electron Microscopy (SEM), and Transmission Electron Microscopy (TEM), were utilized to analyze the purity and structural properties of the synthesized CNTs. The results indicate that higher volumetric flow rates reduced CNT diameters, while thicker catalyst films led to larger diameters. Furnace temperature had a significant influence on the diameter of CNTs synthesized through both gaseous and liquid CVD methods, with the ethylene CVD process yielding the narrowest diameter distribution. Additionally, the effect of reaction time on CNT growth was examined, revealing a major influence on vertical growth rates but no significant impact on tube diameter. These findings provide valuable insights into optimizing CVD parameters to produce high-quality CNTs with potential applications in nanotechnology and materials science.

Keywords: Carbon Nanotubes; Chemical Vapour Deposition; Optimization; Characterization; Structural Properties.

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A Theoretical Investigation into the Potential of N-type Conducting Polymer (BBL) as a Gas Sensing Material for NH_3 and H_2S Detection

Sonu Sunny, Sushri Soumya Jena, Arnab Hazra, Mohit Garg and Sarbani Ghosh*

Department of Chemical Engineering, Birla Institute of Technology and Science (BITS), Pilani Campus, VidyaVihar, Pilani, 333031, Rajasthan, India

*Corresponding Author E-mail: sarbani.ghosh@pilani.bits-pilani.ac.in

ABSTRACT

Recently, conducting polymers (CPs) have emerged as a promising candidate for gas sensing materials because of their structural flexibility, low-cost synthesis, simple manufacturing, and enhanced performance at room temperature. Gas sensors that are based on p-type CPs and their composites have been extensively studied for gas sensing because of their improved stability at ambient conditions. However, they often have limitations in terms of selectivity and sensitivity in reducing gases, especially in detecting the gases at ambient conditions. This study focuses on BBL (benzimidazobenzophenanthroline), which is a widely studied n-type polymer, as the active material for detecting two reducing gases, ammonia (NH_3) and hydrogen sulfide (H_2S), theoretically. In our study, we used molecular dynamics (MD) simulation and density functional theory (DFT) to analyze the adsorption behavior and selectivity of NH_3 and H_2S in the BBL film. Our findings indicate that BBL exhibits significant adsorption of ammonia gas compared to hydrogen sulfide gas while maintaining the integrity of the polymer film's crystallinity in terms of $\pi - \pi$ stacked crystallites. According to our DFT calculations, the adsorption energy is -0.32 eV for NH_3 and -0.21 eV for H_2S. In molecular dynamics simulations, it was observed that adsorption occurs in the open voids within the thin films. This helps the polymer films to retain their crystalline structure. As a result, when reducing gases are detected, the free electrons generated can easily move through the $\pi - \pi$ stack network. The detailed theoretical insights from this study suggest that the n-type conducting polymer, BBL, has the potential to be used as an active material for detecting reducing gases.

Keywords: Organic electronics; Gas sensing; Conducting polymers; MD simulations; BBL Polymer.

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Luminescence and Energy Transfer Studies of Gd^{3+} and Eu^{3+} codoped $LaNbO_4$ phosphor for Solid State Lighting Applications

Muralidaran K, Nitesh Kumar M, Samuel P*

Department of Physics, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamil Nadu - 632014, India.

*Corresponding Author E-mail: samuel.p@vit.ac.in

ABSTRACT

In the illumination and energy fields, white light-emitting diodes (w-LEDs) have become a major light source as they possess long lifetime, high illumination efficiency, brightness, highly reliable and environmentally friendly. Lanthanum niobate ($LaNbO_4$) with a band gap of about 4.8 eV, is a promising oxide material for multifunctional applications. When doped with rare earth ions, $LaNbO_4$ can transfer their absorption energy to the activators and exhibit strong fluorescence. Among them, europium (Eu^{3+}) ions are widely used as luminescence activators for inorganic phosphors that belong to the main red emissive component and have become increasingly essential in producing phosphor converted white LEDs (pc-WLEDs). To enhance the red emission in Eu^{3+} doped $LaNbO_4$, we adopted energy transfer mechanism using Gd^{3+} ion as the sensitizer. As the first step, $La_{(1-x)}NbO_4:Gd_x$ with different amounts of Gd^{3+} (x = 1, 3, 5, 7, 9 and 11 %) ions were synthesized using solid-state reaction technique. Optimum Gd^{3+} concentration was estimated by emission studies. With fixed optimum Gd^{3+} concentration, Gd^{3+} and Eu^{3+} codoped $La_{(1-x-y)}NbO_4:xGd^{3+}/yEu^{3+}$ (y = 1, 3, 5, 7, 9 and 11%) was prepared by varying Eu^{3+} concentration as mentioned. The XRD studies confirmed the phase and purity of all the prepared compounds. The vibrational and absorption nature was observed from the FTIR and reflectance spectra respectively. The Gd^{3+} emission spectra fall in broad blue emission range with its peak at 325 nm due to the transition of $^6P_{7/2}$ – $^8S_{7/2}$ upon the excitation at 273 nm, whereas codoped Gd^{3+}/Eu^{3+} phosphors consist of the strong peak at 614 nm (orangish-red emission) corresponding to $^5D_0$ - $^7F_2$ transition of Eu^{3+} ions. When excited at 273 nm, the energy transfer from Gd^{3+} to Eu^{3+} was observed with an increase in red emission at the expense of the blue emission band. Furthermore, the morphology and elemental analysis studies were performed with SEM coupled with EDAX. No impurity was found other than the precursors used. The CIE chromaticity coordinates of codoped $LaNbO_4$ were in the range of orangish-red. Our results show that $LaNbO_4:Gd^{3+}/Eu^{3+}$ phosphors have the potential to be efficient red-emitting materials for lighting and display applications.

Keywords: Sensitizers; Fluorescence; Luminescence; Phosphor.

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PDMS/ β-phase Si_3N_4 Based Polymer Micro composite as Plantar Pressure Sensor and Energy Harvesting Layer

Anu Chalil[1], Vivek Venugopal[3], Sreenidhi Prabha Rajeev[1,2,*]

[1]*Department of Electronics and Communication Engineering, Amrita Vishwa Vidyapeetham, Amritapuri, India,*

[2]*Centre for Flexible Electronics and Advanced Materials, Amrita Vishwa Vidyapeetham, Amritapuri, India*

[3]*Department of Electronics and Communication Engineering, Amrita Vishwa Vidyapeetham, Bangalore, India*

*Corresponding Author E-mail: sreenidhipr@am.amrita.edu

ABSTRACT

The development and fabrication of sensors are crucial steps in the design of wearable and portable electronic devices which are widely used in the area of medicine and health monitoring. In the current work, a pristine polydimethylsiloxane elastomer (PDMS) based flexible pressure sensor was fabricated. The performance of triboelectric nanogenerators (TENGs) was improved by inclusion of microparticle, **β**-Si_3N_4, to form polymer micro composite with pristine PDMS. The fabricated pressure sensor consists of three layers: a top and bottom copper electrode layer and one dielectric PDMS+ **β**-Si_3N_4 layer. The devices were tested under manual and mechanised tapping methods to generate electrical energy for studying the triboelectric effects and voltage generation capability. The maximum output voltage of 4.72 V is shown for PDMS with 10% **β**-Si_3N_4 composition. The output power density is displayed as 28.79 mW/m^2 at 330 Ω. The sensor was placed on the foot to measure plantar pressure during the experimental validation process and collected average output voltage from individuals of different body weights. This sensor can be deployed at various pressure sensing points at the foot for diagnosing diseases related to plantar pathologies.

Keywords: Flexible pressure sensor; Triboelectric nanogenerator; Polymer micro composite; PDMS+ **β**-Si_3N_4 layer; Plantar pressure.

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Multiwall Carbon Nanotube/Fe_2O_3 Modified Screen Printed Electrode for Electrochemical Detection of Creatinine

Jeethu Raveendran[1], Jagadeesh Bayry[1], P Abdul Rasheed[1, 2*]

[1]*Department of Biological Sciences and Engineering, Indian Institute of Technology Palakkad, Palakkad, Kerala, India- 678623*

[2]*Department of Chemistry, Indian Institute of Technology Palakkad, Palakkad, Kerala, India-678623*

*Corresponding Author E-mail: abdulrasheed@iitpkd.ac.in

ABSTRACT

In healthcare settings, levels of creatinine in body fluids are regarded as vital indicator for the assessment of kidney disease. Easy-to-use, affordable, and accessible electrochemical non-enzymatic screen-printed biosensors have taken the place of complex, traditional enzyme-based assays for this study. A carbon slurry made of Fe_2O_3 and multiwall carbon nanotubes is printed to carbon electrodes that are made in-house with screen printing technique. The oxidation of creatinine in phosphate buffer solution demonstrated a high degree of electrocatalytic activity on the modified sensor. Energy dispersive X-ray analysis and scanning electron microscopy were used to examine the surface morphology and linear sweep voltammetry and differential pulse voltammetry were employed to examine the electrocatalytic activity of the sensor. With a high regression coefficient (R^2=0.997), the creatinine biosensor exhibits a linear detection range of 3 to 24 mM. The detection limit of the sensor was found to be 1.5 mM. Artificial urine samples spiked with creatinine were used to test the suitability of the sensor for real sample exploration. The proposed electrode provides an appealing alternative for enzymatic catalysis in routine creatinine sensing. We anticipate broad use for the creatinine biosensor in the medical and healthcare domains, particularly for onsite medical examinations and at-home testing.

Keywords: Creatinine Sensor; Electrochemical Detection; Screen printed electrodes.

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Sustainable Precision Drilling of 15.5mm Thick Nimonic 263 Plates Using Optimized Abrasive Water Jet Processing

Deepak Chandran Ganesh* and Balaji Vasudevan

Department of Mechanical Engineering, Vel Tech Rangarajan Dr. Sagunthala R&D Institute of Science and Technology, Avadi, Chennai-62, India.

*Corresponding Author E-mail: deepakchan99@gmail.com

ABSTRACT

Abrasive Water Jet (AWJ) processing is emerging as a sustainable and efficient method for machining hard-to-process superalloys like Nimonic 263, aligning with advancements in materials science and environmentally friendly manufacturing practices. In this study, L27 orthogonal array was employed for conducting the drilling experiment on 15.5mm thick Nimonic 263 plate, with Stand-Off Distance (SOD), Water Jet Pressure (WJP), and Abrasive Flow Rate (AFR) identified as key input parameters. SOD was found to have the greatest influence on hole quality. Output parameters such as top and bottom overcut, entry and exit hole diameters, taper, radial overcut, surface roughness, and machining time were measured and analyzed. Detailed morphological analysis was conducted using AFM, SEM, and digital microscopy. Optimal performance was achieved with AFR at 550 g/s, WJP at 360 KPa, and SOD at 1.5 mm, leading to high-quality hole drilling with minimal taper and superior surface finish. An increase in both AFR and WJP values at the optimized SOD demonstrated highly efficient drilling, reducing machining time. This study highlights the potential of AWJ as a sustainable, environmentally conscious process for creating precise holes in thick Nimonic 263 plates, with applications in aerospace, gas turbines, advanced heat exchangers, and high-temperature fluid control systems, where precision, reduced material waste, and thermal efficiency are critical.

Keywords: Abrasive Water Jet Drilling; Nimonic-263 Surface Roughness; Aerospace; Precision Drilling.

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Niobium Mxene Modified Carbon Felt Electrode for Capacitive Deionization in the Removal of Cr^{6+} from Metal-Bearing Water

Hibu Munku[1], Gouri J S[2], P Abdul Rasheed[1], Shibu K[2], Praveena Gangadharan[1,*]

[1] *Environmental Science and Sustainable Engineering Centre, Indian Institute of Technology Palakkad, Kerala, India- 678623*

[2] *Department of Civil Engineering, College of Engineering Trivandrum, Kerala, India-695016*

*Corresponding Author E-mail: praveenag@iitpkd.ac.in

ABSTRACT

Hexavalent chromium (Cr^{6+}) has been recognized as a carcinogenic and mutagenic heavy metal, exposure to it can be hazardous, potentially causing significant adverse health effects. Capacitive deionization (CDI) has gained major attraction as a viable technique for deionization and desalination operations due to its advantages such as low operating voltage, low cost, simple construction, and less production of secondary pollutants. In this study, Niobium MXene (Nb_2CT_x,) was coated onto carbon felt (CF) electrode for the CDI system and investigated the capacity for the removal of Cr^{6+} from the wastewater. Owing to unique properties like large surface area, hydrophilicity and excellent stability MXene has been used for enhancing the efficiency of electrodes. The Nb_2CT_x was synthesized through etching from its precursor Nb_2AlC MAX phase with hydrofluoric acid and was thoroughly characterized. The MXene-coated electrodes were electrochemically characterized and used as the cathode of the deionization system. The removal efficiency of Cr^{6+} was studied under various conditions including applied voltages, pH levels, and initial concentrations Cr^{6+}. For comparison purposes, CDI system with bare CF electrodes symmetric system (CF||CF) was analyzed parallelly. As the result demonstrated, superior electrochemical reduction capacity was observed in MXene-coated electrodes asymmetric system (CF||Nb_2CT_x) leading to the efficient conversion of toxic Cr^{6+} to Cr^{3+} ions at an acidic pH 2. The asymmetric system exhibits a remarkable removal efficiency of 94% for Cr^{6+} at a lower applied potential of 1.5V within 2 hours, highlighting the energy conservation aspect of the developed system. Furthermore, asymmetric system outperformed symmetric system in terms of charge transfer and also showed excellent cycle stability up to five cycles of operation.

Keywords: Capacitive deionization; Niobium MXene; Carbon felt; Hexavalent chromium; Wastewater treatment.

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An Electrochemical Sensor for the Detection of Chloride Ions Using Disposable Screen-Printed Silver Electrodes for Multitude Samples with Portable Potentiostat

Anson T Mathew[1], Pooja Das M[2], Jeethu Raveendran[1]

[1]*Department of Biomedical Engineering Sahrdaya College of Engineering and Technology P.B. No 17, Kodakkara, Thrissur, Kerala, India*
[2] *APJ Abdul Kalam Technological University, Thiruvananthapuram, India*

*Corresponding Author E-mail: jeethu@sahrdaya.ac.in

ABSTRACT

Real-time detection and measurement of chloride ion concentrations are vital across various industries, including wearable healthcare devices and environmental pollution control. Monitoring chloride levels in water is crucial for safeguarding public health, protecting the environment, and ensuring compliance with water quality regulations in industrial and agricultural applications. To address this need, we developed a low-cost chloride sensor that can be screen printed on PET sheets using conductive silver paste and silver chloride paste. The sensor's performance was evaluated through potentiometric measurements, utilizing an auxiliary Ag/AgCl reference electrode and a carbon electrode. Cyclic voltammetry was employed to assess the chloride sensing capabilities. A variety of samples with different chloride concentrations were tested, confirming the sensor's effectiveness. The detection limit was established at 200 µM, with a measurement range extending up to 100 mM. The sensor exhibited strong sensitivity and linearity, with an R^2 value of 0.9764. This innovative method provides a convenient and cost-effective solution for rapid chloride ion detection and monitoring, making it an ideal option for remote applications. Overall, the development of this sensor represents a significant advancement in the field of water quality monitoring, facilitating timely identification of potential issues and contributing to better regulatory compliance and environmental protection.

Keywords: Chloride sensor; Water quality; cystic fibrosis; Electrochemical sensor; Portable Potentiostat.

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Unravelling Structural Transformations and Degradation Mechanisms of Pb-Sn Mixed Perovskite Thin films

Shana Sudhakaran, Vinod E Madhavan*

Department Of Materials Science and Engineering, National Institute of Technology Calicut, Kozhikode, Kerala 673601, India.

*Corresponding Author E-mail: vinodem@nitc.ac.in

ABSTRACT

Perovskite solar cells (PSCs) have attracted a lot of attention due to their potential to transform the photovoltaic industry with higher efficiency and lower material usage. However, their intrinsic instability under conditions such as moisture, light, and heat poses a significant obstacle to their growth, making them unsuitable for long-term use. $MAPbI_3$ (MAPI, x = 0) is the most studied compound for PSC applications, however, the presence of Pb causes toxicity. $MASnI_3$ (MASI, x=1) is a potential replacement for this compound to avoid toxicity concerns. In this study, new compounds of six different families of perovskites are designed to reduce the Pb content by systematically increasing the presence of Sn. Pb-Sn binary perovskite thin films ($MAPb_{(1-x)}Sn_xI_3$ [$0 \leq x \leq 1$]) were prepared and crystallized at an annealing temperature of 110 °C for 1 hour, and properties were investigated under ambient conditions. The surface morphology of the freshly prepared MAPI shows a well-defined grain with 500–1000 nm grains, whereas the MASI (x = 1.0) shows a mud-flake morphology. With the replacement of Pb by Sn in $MAPb_{(1-x)}Sn_xI_3$, the optical bandgap is found to be varying between 1.55 eV and 1.78 eV. All samples form well-defined tetragonal phases with varying peak intensities in XRD. The compound with x = 0.8 shows sharp and high-intensity peaks, representing the presence of higher grain formation and crystallinity. To gain a deeper understanding of their degradation mechanisms and structural transformations, samples were left at ambient conditions with 40–60 RH. An analysis of all compounds reveals that phases containing mixtures of Sn and Pb (x = 0.2 to 0.8) exhibited a more stable morphology, even after 28 days, compared to the pristine compounds. This must be due to the increased presence of Sn, resulting in an improved tolerance to moisture in the compound, which is a main breakdown mechanism for MAPI. This study provides a basis for the creation of focused strategies to improve the stability of Pb-based perovskite materials by incorporating Sn, bringing them one step closer to actual application in clean energy generation.

Keywords: Perovskite; $MAPbI_3$; Thinfilm; Solar cells; Stability.

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Synthesis of Copper doped Tin Oxide Thin Films for Hydrogen Gas Sensing

Dylan Daniel Muruppel*, C Sneha, Soney Varghese

Department of Materials Science and Engineering, NIT Calicut, P.O. 673601, Kozhikode, India

*Corresponding Author E-mail: dylandmuruppel@gmail.com

ABSTRACT

This study investigates the synthesis and characterization of tin oxide (SnO_2) thin films co-sputtered with copper (Cu) for efficient hydrogen gas sensing. The integration of metal oxides like Tin Oxide in gas sensors is well-established due to their high sensitivity and low cost. The approach involves doping SnO_2 with different concentrations of Cu (sputtering time of 20, 30 and 40 seconds) to enhance sensor performance, particularly for hydrogen detection and to study the changes with doping concentration. Characterization techniques including Scanning Electron Microscopy (SEM), X-Ray Diffraction (XRD) and Wettability tests confirm the presence of Tin Oxide and Copper, and confirms the porous, more hydrophobic nature of the thin films which is crucial for optimal hydrogen gas sensing. EDS (Energy Dispersive System) data confirms the increase in Cu content from 2.8% to 3.8 % in the 20 to 40 second samples. UV-Visible Spectroscopy data indicates that Copper doping reduces the Band-Gap Energy of Tin Oxide and further decreases with increase in Cu doping (3.4429eV to 3.3315eV), enabling improved conductivity. Temperature v/s Resistivity results indicate that the film maintains Semiconductor properties and exhibits better thermal stability with increase in Cu doping. The 40 second doped sample showed a response percentage of 0.88%, far superior to that of the undoped sample with 0.12%. The doped sample also presented rapid response and recovery times of 20 and 35 seconds respectively. These materials have significant implications for the development of cost-effective, high-performance hydrogen sensors in energy, environmental, and healthcare applications, contributing to safer and more efficient industrial processes.

Keywords: Hydrogen Gas Sensing; Tin Oxide Thin Film; Copper Doping.

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Synthesis and Characterisation of Blue Emitting TADF Emitter with Electron Transporting Capability

Manmohan Dash[1,*], M N Satyanarayan[1], Jayathirtha Rao Vaidya[2], Godumala Mallesham[3]

[1]*Optoelectronics Lab, Physics Department, National Institute of Technology Karnataka, Surathkal, Mangalore, 575025, India*

[2]*CSIR - Indian Institute of Chemical Technology, Uppal Road Tarnaka, Hyderabad-500007, India*

[3]*Department of Chemistry, Anurag University, Hyderabad, Telangana, 500088, India*

*Corresponding Author E-mail: mdash.197ph008@nitk.edu.in

ABSTRACT

Thermally Activated delayed fluorescence (TADF) based emitters are an attractive alternative to producing high efficiency organic light emitting diodes. Among the TADF emitters, those emitting blue light and also possessing good charge transport properties are highly sought after. In this work, the synthesis and characterisation of a blue TADF emitter with good electron transport capabilities is presented. The blue TADF emitter is produced by appending triphenyl-phosphineoxide, $Ph_3P = O$ (an electron transport enhancer) to the pyrene (Carbazol based) derivatives. Through impedance spectroscopy, it is inferred that the TADF emitter has better electron transporting capability than some standard electron transport materials (TAZ), similar to some others (AlQ3), slightly inferior to some (TPBi) and 2 order of magnitude smaller than some (BPhen). Alongside, the thermal, electrochemical, photophysical and morphological studies have been carried out on the TADF emitter, which will be discussed in the presentation.

Keywords: Pyrene Phosphine Oxides; Thermally Activated Delayed Fluorescence (*TADF*); Impedance Spectroscopy; Electron Transport in Organic Semiconductors.

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Polymer Nanocomposite for Piezoelectric Nanogenerators and Pressure Sensors: Impact of Morphology and Surface Charge of Nanofiller on the Polymer Matrix

Ankur Verma[1,3], Pritha Dutta[1,2], Ashutosh Kumar Singh[1,2,3], Subash Cherumannil Karumuthil[1,2,3,*]

[1]*Center for Nano and Soft Matter Sciences, Bengaluru, 562162, India*

[2]*Manipal Academy of Higher Education, Manipal 576104, Karnataka, India*

[3]*Academy of Scientific and Innovation Research (AcSIR), Ghaziabad Uttar Pradesh, 201002, India*

*Corresponding Author E-mail: cksubash@cens.res.in

ABSTRACT

Piezoelectric nanogenerators (PENGs) have emerged as a potential technology for turning mechanical energy into electrical energy at the nanoscale, providing long-term power solutions for self-powered systems. This work investigates the design and performance of a piezoelectric nanogenerator (PENG) made from polyvinylidene fluoride (PVDF), a polymer recognised for its exceptional piezoelectric characteristics. PVDF's piezoelectric property, amplified by mechanical stretching, nanofiller incorporation and electrical poling, makes it an attractive choice for energy harvesting applications.[1,2] The nanogenerator converts mechanical energy, such as vibrations and human motion, into electrical energy. This study uses the addition of various morphology and surface-charged nanomaterial into a PVDF matrix for polymer nanocomposite piezoelectric film with high β-phase crystallinity, which improves their piezoelectric response.[3] The device's performance is assessed by measuring its output voltage and current under various mechanical stress settings. Experimental results suggest that the nanocomposite-based PENG can provide enough electrical output for low-power devices, making it suitable for self-powered sensors and wearable electronics. A prototype device with PDMS hydrophobic coating was used to demonstrate real-time uses of this piezoelectric functional soft material. The optimised combination achieved an impressive power of 4623.8 μW and power density of 377.46 $\mu W/cm^2$ with a load resistance of 1 MΩ. To ensure stability, the prototype was hand-tapped 3000 times continuously. The findings emphasise nanocomposite nanogenerators play a potential role in energy harvesting in portable and sustainable power systems, with more gains likely if material characteristics and device architecture are optimised.

Keywords: Piezoelectricity; Pressure sensors; Nanocomposites

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Ultrasonication-Enhanced Green Synthesis of Biodiesel Using Biochar Catalyst from Cycas circinalis Seed Shells

Vanisree G S, Manikandan, Rahul J, Vignesh M, Aparna K*

Department of Chemical Engineering, National Institute of Technology Calicut, Kerala 673601, India

*Corresponding Author Email: aparnak@nitc.ac.in

ABSTRACT

The urgent need for alternative fuels arises from dwindling fossil fuel reserves and increasing global environmental concerns. Renewable energy must be generated from sources with a smaller ecological footprint. A viable alternative is biodiesel from plant-derived oils and animal fats. In this study, biodiesel was produced from Jatropha oil using ultrasonication-assisted transesterification with a novel Cycas circinalis seed shell biochar catalyst. The catalyst was characterized by XRD, FTIR, SEM, and EDS, while the biodiesel was analysed using 1H-NMR spectroscopy. The process was optimized using central composite design (CCD) based on response surface methodology (RSM). A maximum biodiesel yield of 91.27% was achieved with a catalyst concentration of 2.3 wt.%, a 10:1 methanol to oil ratio, 38 minutes of reaction time, and a reaction temperature of 52°C.

Keywords: Biodiesel; Cycas circinalis Seed shell; Jatropha oil; Transesterification; Heterogeneous catalyst; Biochar.

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Study of Microstructure and Mechanical Properties of Wire Arc Additive Manufactured (WAAM) Inconel 625 Hollow Cylinder using Cold Metal Transfer (CMT)

Athul Krishna P B[1], Navin V Varughese[1], Adhith P Omanakuttan[1], Dil Binu[1], Anoop K Unni[2,*]

[1] *Department of Metallurgical and Materials Engineering, Amal Jyothi College of Engineering, Kanjirappally, Kerala, 686518, India.*

[2] *Assistant Professor, Department of Metallurgical and Materials Engineering, Amal Jyothi College of Engineering, Kanjirappally, Kerala, 686518, India*

*Corresponding Author E-mail: anoopkunni@amaljyothi.ac.in

ABSTRACT

This study investigates the potential of Cold Metal Transfer Wire Arc Additive Manufacturing (CMT-WAAM) as an alternative to conventional methods for producing Inconel 625 hollow cylinders. Inconel 625, a nickel-based superalloy known for its high-temperature strength and corrosion resistance, is widely used in critical applications. Traditional manufacturing techniques often face limitations related to design flexibility and material waste, whereas CMT-WAAM offers precise material deposition with minimal heat input and reduced waste. The current research focuses on the fabrication of hollow Inconel 625 cylinder by optimizing process parameters and applying heat treatments, such as normal and solution annealing to evaluate microstructural evolution, micro-tensile properties, and Vickers microhardness in both as-welded and heat-treated conditions. The results indicate that the ultimate tensile strength (UTS) was found higher in the top region than the bottom region in as-welded samples, while annealing contributed to a decrease in UTS. Additionally, significant hardness variations were observed along the build direction, with as-welded samples exhibiting higher hardness compared to heat-treated samples. These results highlight how important it is to improve the mechanical properties of Inconel 625 components by tailoring CMT-WAAM parameters and suitable post-processing methods.

Keywords: Wire Arc Additive Manufacturing; Cold metal transfer; Inconel 625; Microtensile; Heat treatment; Solution annealing.

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WS_2/NiS_2 Based Heterostructures Grown on Nickel Foam as an Electrocatalyst for Efficient Hydrogen Evolution

Arunya Raj R, Nabeel N A, Aswathi G*

Department of Physics, National Institute of Technology Calicut, NIT Campus (P.O.), Kozhikode-673 601, Kerala, India.

*Corresponding Author E-mail: aswathig@nitc.ac.in

ABSTRACT

Hydrogen is considered as a clean energy source in the transition to sustainable energy. It can serve as a secondary energy carrier, storing and delivering energy that was initially generated from renewable resources like solar or wind. Water electrolysis by renewable energy sources is considered as one of the primary methods for producing green hydrogen in the future. In the case of electrocatalytic water splitting, precious metals like Pt, Ir, Ru and their alloys are considered as the most effective electrocatalyst in terms of activity and stability. However, their scarce availability and high cost have limited their practical use on an industrial scale. Transition metal chalcogenides (TMCs) show great potential as earth-abundant electrocatalysts for water splitting, offering a promising alternative to noble metals. TMCs show unique chemical and physical properties which can be optimized by tuning the nanoarchitecture or electronic properties. The strategic design and development of heterogeneous electrocatalysts for the hydrogen evolution reaction (HER) has become a prominent research focus nowadays, yet reports on practical and pH-universal tungsten disulfide (WS_2)-based hybrid composites remain scarce. Herein, we propose a novel catalyst (WS_2/NiS_2) grown on Nickel foam, flexibly applicable to all pH electrolytes. The influence of heterojunction of the catalyst on HER (Hydrogen Evolution Reaction) is investigated. The synergistic effects of the heterojunctions are optimized by modifying the ratio of the heterojunction components. Thus, this work provides new insights into WS_2 based hybrid materials potentially applied to sustainable energy.

Keywords: Hydrogen evolution reactions (HER); Transition metal Chalcogenides (TMCs); WS_2-based, heterojunction.

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Prediction of ABO_3-type Perovskite Structures using Machine Learning for Developing Microwave Dielectric Ceramics

Sukruth Rameshkumar, Fayas Shani, Asish Issac Alex, Mohammed Rashad*

Department of Mechanical Engineering, National Institute of Technology Calicut, Kozhikode, Kerala 673601, India

*Corresponding Author E-mail address: rashad@nitc.ac.in

ABSTRACT

Microwave dielectric materials have a significant impact on our everyday lives, serving a broad spectrum of applications in wireless communication devices, from satellite communications to GPS and telecommunications. To meet the requirements of current and future systems, new microwave components utilizing specialized dielectric materials and innovative designs are necessary. The recent advancements in microwave telecommunication have resulted in an increased interest in device miniaturisation by developing dielectric resonators (DRs) with high dielectric constants and low dissipation factors. Oxide perovskite ceramics have attracted increasing interest as DRs due to their tunable structures to meet the required microwave characteristics. Developing perovskite with the desired properties is a complex task, where classical theory and density functional theory are heavily utilized to predict the dielectric constant based on its chemical composition. With the advancement of machine learning techniques, researchers have predicted the properties, especially the dielectric constant of perovskite ceramics. In the present study, a novel predictive modelling approach was employed wherein the properties, namely dielectric constant and quality factor of existing perovskites, reported in the literature, were utilised to predict the structure of a new perovskite ceramic having the desired properties. With the use of Extreme Gradient Boost (XG Boost) and Categorical Boost (CatBoost) algorithms, the radii of the two sites, A & B in the ABO_3 perovskite is predicted, to match the dielectric constant and quality factor of the desired ceramic. A separate code was developed to predict the stoichiometric ratio of cations which could occupy each site. Two sample sets of dielectric constants (60,90) and quality factor value, (100000) required for a prospective DR application are selected, and by using them the model could predict two new perovskite structures, $Ca_{0.5}Sr_{0.3}Ba_{0.2}Zi_{0.2}Ti_{0.8}O_3$ and $SiSr_{0.3}Ti_{0.7}O_3$. The phase formation of the predicted oxide perovskite structures was experimentally validated by the solid-state sintering route followed by XRD analysis. The developed model will be useful for selecting DR materials for various microwave applications with dielectric constant within the range of 60 to 90.

Keywords: Machine Learning; Perovskite; Dielectric resonator; Ceramics; Prediction

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Numerical Modelling of Semi-Solid Flow in Solidifying Mixtures to Capture Shear Bands

A Tamrakar[1], U Godwal[1,2], S Bhagwath[2,3], B Gaffari[4], M Li[4], P D Lee[2,3], S Karagadde[1,*]

[1]*Department of Mechanical Engineering, Indian Institute of Technology Bombay, Mumbai, India*

[2]*Research Complex at Harwell, Harwell Science & Innovation Campus, Didcot OX11 0FA, UK*

[3]*University College of London, WC1E 6BT, UK*

[4]*Ford Research and Advanced Engineering, Dearborn, USA*

*Corresponding Author E-mail: s. karagadde@iitb.ac.in

ABSTRACT

Semi-solid flow (SSF) of solidifying mixtures occurs in manufacturing processes, volcanic magma flow, and food processing industries. The thermo-mechanical response of the semi-solid mushy zone under deformation is reported to play a key role in the formation of bands of defects, including pores. As an illustrative example, in metallic castings, improved knowledge of the complex interaction of solid-liquid phases, grain growth kinetics, permeability development and rheological properties of semi-solid material that contain externally-solidified crystals will help develop more realistic models. To do this a macroscopic model was developed that captures the SSF behaviour in shear strain localization during porous media flow to predict the shear band locations. The variation in permeability due to discontinuities in solid fraction ratio values was modelled using previously developed empirical relations. From numerical simulations it is evident that with an increasing solid fraction ratio, localized high shear strain rate magnitudes decrease and shift away from center. These findings highlight the potential to apply the principles and modeling approaches previously developed in granular mechanics to mentioned applications. They also suggest that possible benefits might be gained from exploring and exploiting further synergies between these fields.

Keywords: Semi-solid flow; Defect bands; Anisotropic permeability.

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Biodegradable Food Packaging

Arya A*, Keerthana V, Diya T K
Chemical Engineering Department, Government Engineering College,Thrissur,India
*Corresponding Author E-mail: aryaajessh23@gmail.com

ABSTRACT

This study explores the feasibility of producing cost-effective and environmentally friendly packaging using a composite blend of polylactic acid (PLA), bagasse, tannin, and amylase. With the rising demand for biodegradable packaging to mitigate environmental pollution and reduce landfill waste, bioplastic materials have gained prominence. However, PLA, one of the most common bioplastics, has limitations in terms of cost and decomposition rate, often requiring industrial composting conditions to break down effectively. By incorporating natural additives and fillers, this research aims to enhance both the economic and functional viability of PLA-based biodegradable packaging. Bagasse, a fibrous byproduct of sugarcane, serves as an economical and sustainable filler material, reducing the dependency on PLA while retaining the necessary structural integrity for packaging applications. As an abundant, low-cost agricultural residue, bagasse also improves the overall rigidity and heat resistance of the material. Replacing a significant portion of PLA with bagasse could decrease material usage and costs substantially without compromising quality, thereby making the packaging solution more affordable for large-scale production. Additionally, tannin—a plant-derived polyphenol known for its antimicrobial and antioxidant properties offers benefits for product shelf life by preventing premature microbial degradation. Tannin's inherent water resistance also enhances the packaging's durability under normal use, yet it remains biodegradable once exposed to appropriate environmental conditions. Its application as a surface coating or minor additive provides functionality while maintaining cost-effectiveness. The inclusion of amylase, a starch-degrading enzyme, addresses one of the most significant challenges in biodegradable packaging: controlled and efficient decomposition. Amylase accelerates the breakdown of starch in bagasse, thus triggering faster microbial activity and speeding up the decomposition process under moist conditions, such as those in composting or landfill environments. However, since amylase could activate prematurely in humid conditions, careful management techniques are necessary to ensure it remains inactive until disposal. Encapsulation or layering strategies could protect the enzyme, thereby enabling controlled activation. By using amylase sparingly, the packaging material can maintain stability during its functional life and rapidly decompose upon disposal. In conclusion, a PLA-bagasse-tannin-amylase composite provides an economically viable solution that balances durability, controlled degradation, and eco-friendliness. Such a material can meet consumer demand for sustainable packaging without substantial cost increases, particularly for industries prioritizing sustainability. This approach demonstrates the potential of using natural fillers and additives to create high-performance, biodegradable packaging suitable for a wide range of applications, thereby promoting a shift toward more sustainable packaging solutions.

KEYWORDS: Biodegradable; Cost effective; Environmental friendly; Anti-microbial; Antioxidant.

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Non-Invasive Ketosis Detection via Breath Acetone using a Quartz Tuning Fork Sensor Array

Satyendra Vishwakarma and Suwarna Datar*

Department of Applied Physics, Defence Institute of Advanced Technology, Pune 411025, Maharashtra, India

*Corresponding Author E-mail: suwarnadatar@gmail.com

ABSTRACT

The study of human health through breath biomarkers has emerged as a significant area of research, offering a non-invasive approach to daily health monitoring and early disease detection. Human exhaled breath contains a wealth of biochemical information that reflects various physiological and pathological conditions. Among the numerous biomarkers found in breath, acetone holds significant promise for detecting metabolic states, particularly ketosis. Ketosis is characterized by elevated levels of ketone bodies, including acetoacetate (AcAc), β-hydroxybutyrate (BHB), and acetone. This metabolic state occurs when glucose availability is limited, prompting the body to break down fatty acids for energy production. Ketosis can arise from factors such as starvation, ketogenic diets, and pathological conditions like heart failure, diabetic ketoacidosis, and euglycemic ketoacidosis. Therapeutic ketosis, in which elevated BHB levels replace glucose as the primary energy source, has demonstrated benefits in conditions such as Alzheimer's disease, Parkinson's disease, epilepsy, and type 2 diabetes. Regular monitoring of ketone levels is crucial in both clinical and dietary settings. Acetone, a highly volatile compound, shows a strong correlation between blood BHB levels and breath acetone concentrations. Breath acetone levels in the range of 2 to 40 ppm have been identified as an indicator of ketosis, and its measurement can aid in managing nutritional choices and therapeutic interventions. In this study, we aim to detect acetone concentrations ranging from 1 to 100 ppm using an array of quartz tuning fork (QTF)-based sensors in exhaled breath. The sensor was fabricated using a polymer matrix incorporating nanomaterials as additives. The nanomaterials were synthesized via the laser ablation technique and characterized through X-ray diffraction (XRD), UV-Visible spectroscopy (UV-Vis), and transmission electron microscopy (TEM). Three types of nanomaterials; zinc oxide (ZnO), copper (Cu), and silver (Ag) were developed and embedded into the polymer. The results will be correlated with blood ketone levels to validate the accuracy and reliability of the sensor. By developing a reliable, non-invasive method for monitoring ketosis, this research has the potential to improve the management of metabolic diseases and conditions influenced by ketosis. The proposed breath acetone sensor array offers a convenient alternative to traditional blood tests, enhancing patient outcomes through better dietary management and timely therapeutic interventions.

Keywords: QTF sensor; Acetone; Ketosis; Non-invasive.

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Tuning the Photoresponse Properties of Poly(3-hexylthiophene) by Doping with Organic Dyes

Aswin Ramesh and **C S Suchand Sangeeth***

Department of Physics, National Institute of Technology Calicut, Calicut- 673601, Kerala, India

*Corresponding Author E-mail: sangeeth@nitc.ac.in

ABSTRACT

Poly(3-hexylthiophene) (P3HT) is a widely used organic semiconductor material which finds applications in organic field effect transistors, organic light emitting diodes and organic solar cells. Tuning the photoresponse properties of P3HT is crucial in improving the performance of these devices. In this study the charge transport properties of dye doped P3HT films are investigated under dark and light illumination We used N,N′-Bis(3-pentyl)perylene-3,4,9,10-bis(dicarboximide) and Perylene-3,4,9,10-tetracarboxylic dianhydride, Pigment Red 224 dyes for doping. P3HT-Perylene film mixed at different ratios was spin coated on ITO and silver was evaporated to make the top contact. The interaction between p-type P3HT and n-type perylene system results in a charge transfer complex with improved electronic properties compared to the individual materials. This enhanced charge transport ability makes the P3HT perylene system a promising candidate for high-performance organic electronic devices. The perylene doped P3HT films showed more than an order higher conductivity as compared to the bare P3HT films. In addition to its superior charge transport, the P3HT perylene charge transfer system also exhibits strong light absorption and efficient energy transfer properties. This work entails both the photoresponse study and the transport characteristics of the blend. The transport mechanism is corroborated using dc conductivity and frequency dependent ac conductivity measurements to understand the nuances of transport in the blend system. The improved photoresponse characteristics make it well-suited for photovoltaic applications and the fundamental understanding of the system is necessary to fine tune the material towards solar cell applications.

Keywords: P3HT; Photoresponse; Perylene; Charge transport.

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High-Performance Polyvinyl Alcohol-Based Ternary Nanocomposites with Enhanced Thermal and Mechanical Properties for Flexible Device Applications

Shasiya P S[1], Soney Varghese[2], Ajalesh B Nair[1,*]

[1]*Department of Chemistry, Union Christian College, Aluva, Kerala, India*

[2]*Department of Materials Science and Engineering, NDRL, National Institute of Technology, Calicut*

*Corresponding Author E-mail: *ajaleshbnair@uccollege.edu.in*

ABSTRACT

The exploration of robust and flexible polymer nanocomposites is gaining interest as a modish class of substance with promising angles on diverse applications. Herein, we demonstrate a strategy for developing a ternary polymer nanocomposite system based on Graphene Oxide (GO) and Polyhedral Oligomeric Silsesquioxane (POSS) along with PVA employed by facile solution casting method. The results of different substantial characteristics were evaluated using X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), Universal testing machine (UTM), and Thermogravimetric analysis (TGA) respectively. FTIR analysis confirms the interaction between the POSS/ GO filler and the PVA matrix. X-ray diffraction data clearly show a significant improvement in the crystallinity of nanocomposites with an increase in the GO fillers. The scanning electron micrographs confirmed the homogeneous distribution of fillers in the PVA matrix. Thermogravimetric measurements revealed that the nanocomposite films exhibited improved thermal stability. With the addition of GO/POSS to PVA, mechanical properties including tensile strength and Young's modulus were significantly enhanced. The improved mechanical strength and enhanced thermal stability of these systems paved a new paradigm for the simple and economic route for polymer-based flexible devices.

Keywords: Nanocomposites; PVA; POSS; Graphene Oxide; Flexible devices.

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Growth and Characterization of Aluminum Nitride (AlN) Thin film on Steel using Plasma Enhanced Chemical Vapor Deposition Technique

Amit Bhargav*, Abhishek Bhaisare, C Sasikumar, Mangesh Lodhe, and Sanjay Shrivastava

[1]*Department of Materials and Metallurgical Engineering, Maulana Azad National Institute of Technology, Bhopal, India*

*Corresponding Author E-mail: abhargav260@gmail.com

ABSTRACT

Aluminium Nitride (AlN) thin films are deposited on steel using plasma-enhanced chemical vapor deposition (PECVD), exploring their impact on the piezoelectric effect, excellent mechanical properties, chemical inertness, and high melting point. In this study, develop an AlN-coated steel surface and measure its tribological, mechanical, and oxidation behavior. The x-ray diffraction results confirmed the formation of AlN coating and its thickness range in 0.5-1.1 µm measured by scanning electron microscope. The morphology of AlN film is a nano-crystalline structure with a globular shape. The roughness of the thin film was 96.377nm, and the grain size was between 0.073 – 0.213 µm measured by atomic force microscope (AFM). The thin film also exhibited excellent resistance to oxidation and wear.

Keywords: Thin film; Aluminum nitride (AlN) coating; Plasma enhanced chemical vapour deposition (PE-CVD).

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Precipitation and Coarsening Behaviour Study of Different Precipitates on Thermal Ageing of 304HCu SS for Different Periods of Time

Kanhu Charan Sahoo*
Department of Materials Science and Engineering, NIT, Patna Bihar-800005
*Corresponding Author E-mail: kcsahoo.ph@nitp.ac.in

ABSTRACT

304HCu SS is an indigenously developed candidate material for reheater/superheater tubes in Advanced Ultra Super Critical (AUSC) power plant in the temperature range 873-948 K due to its good combination high temperature creep strength, resistance to oxidation and corrosion and better fabricability compared to conventional austenitic stainless steel. It mainly contains around 3 wt. % of copper, certain amounts of niobium, nitrogen and increased carbon content compared to 18Cr-8Ni 304SS for enhancing creep strength. In general, high temperature mechanical properties and the stability of the as received matrix is directly linked to the formation, dissolution and coarsening of the precipitates. Again the formation of incoherent precipitates is not beneficial for good creep strength since it gives higher interfacial strain with the matrix from where cavitation process can start earlier. Hence, it is important to study the microstructural evolution of the steel at the above mentioned temperatures for longer duration. 304HCu SS has been aged for 1200, 5000, 7000 and 24000 hours at 923 K to study the microstructural aspects viz. evolution of new precipitates, coarsening of the existing and new precipitates, distribution of carbides, grain size and their consequence. The frequency distribution of intergranular and intragranular carbides shows increase in size and decrease in number density with increase in ageing time. The size of Cu-particles, examined through Transmission Electron microscopy was found to increase with increase in ageing time and was found to be 20, 30, 50, 80 nm for 1200, 5000, 7000 and 24000-hour ageing time. All the aged specimens have been electrochemically dissoluted to study the evolution of new and existing precipitates through XRD analysis. Different forms of Laves phases have been found for 7000 and 24000 hours' steel. Vickers micro-hardness was done for different thermal aged and it was observed that hardness was found to increase with increase in ageing time.

Keywords: 304HCu SS; Thermal ageing; SEM; TEM; XRD.

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Polyvinylidene Fluoride-Ti_3C_2 MXene Film-Based Flexible Piezoelectric Nanogenerator for Superior Underwater Energy Harvesting

Athira M*, Soney Varghese
Department of materials science and engineering, National Institute of Technology, Calicut, India
*Corresponding Author E-mail: athira_p200117mt@nitc.ac.in

ABSTRACT

Piezoelectric nanogenerators (PENGs) have emerged as a promising technique for harvesting energy from water, notably by absorbing mechanical energy from ocean waves. These devices use the piezoelectric effect to transform mechanical energy into electrical energy, making them suitable for sustainable applications. This study aims to synthesise, characterise, and develop a flexible piezoelectric polymer composite film of polyvinylidene fluoride (PVDF) and Ti_3C_2 utilising a simple solvent casting method that does not need external poling. PVDF is combined with various concentrations of MXene (0.2, 0.8, 1, 2 wt%), followed by solvent casting using DMF. The composite film is analysed using methods such as scanning electron microscopy (SEM), X-ray diffraction (XRD), Raman spectroscopy, Fourier transform infrared spectroscopy (FTIR), and dynamic contact mode electrostatic force microscopy (DC-EFM). Doping Ti_3C_2 nanosheets into the polymer matrix increased the beta(β) phase in PVDF. PVDF doped with 1 wt% MXene has the largest β phase percentage, as well as superior piezoelectric and mechanical properties. MXene is equally dispersed in the PVDF matrix, which increases the β phase while lowering the undesired alpha(α) phase configuration. According to the DC-EFM results, 1wt% MXene incorporated PVDF produces more voltage than other PVDF-MXene compositions. The FTIR spectrum indicates that the β phase has improved. A piezoelectric Nanogenerator was made from PVDF and 1 wt% MXene. It was tested by tapping and found to yield around 5 V of electrical energy. Underwater energy harvesting studies were carried out with water flow rates ranging from 0 to 3 m/s. The output voltage grew with water flow rate to a maximum peak-to-peak voltage of 21 V at a water flow rate of 3 m/s, with short circuit current of 0.9 µA. It is possible to power underwater sensor networks using this device.

Keywords: PVDF-Ti_3C_2 Composite; Piezoelectric Nano-generator; DC-EFM; Flexible device.

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Tribological Performance of FDM-Printed PETG Parts Under Wet Sliding Conditions: Insights for Industrial Applications

Mohan Jayshankar[1], M B Kumbhar[2, *], Asrith Raj[1], T Jagadeesha[1]

[1]*Mechanical Engineering Department, National Institute of Technology, Calicut, Kerala, 673601*
[2]*Mechanical Engineering Department, COEP Technological University, Shivajinagar, Pune-412105*
*Corresponding Author E-mail: mkumbhar44@gmail.com

ABSTRACT

This research investigates the tribological properties of 3D-printed PETG (Polyethylene Terephthalate Glycol) parts fabricated through Fused Deposition Modeling (FDM) under wet sliding conditions. Key parameters, including the coefficient of friction (COF), specific wear rate, and friction force variations over time, were evaluated using a pin-on-disc tribometer with castor oil as a lubricant. Experimental results revealed phenomena such as stick-slip behavior, vibrations, and localized heating, leading to increased wear. Post-test analysis demonstrated reduced surface roughness due to the lubricant's smoothing effect. Findings align with established tribological principles, confirming that wet lubrication reduces COF and wear compared to dry sliding. These insights have direct applications in automotive, robotics, and biomedical engineering, where 3D-printed polymer components are integrated into lubricated gears, bearings, and sliding mechanisms. This research supports the design of lightweight, wear-resistant parts and advances sustainable manufacturing by integrating 3D printing with bio-lubricants.

Keywords: FDM; PETG; Tribology; Coefficient of Friction; Wet Sliding; Surface Roughness; Engineering Applications.

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Synergistic Integration of MoS_2-Ag-TiO_2 in Polyurethane: A Non-Toxic Coating with Enhanced Photocatalytic potential for Anti-biofouling applications

Athira S Vijayan[1], Abey Joseph[2], Baiju G Nair[2] and Sajith V[1,*]

[1]*Department of Materials Science and Engineering, National Institute of Technology, Calicut, NIT Campus PO, Kozhikode, 673601, Kerala, India*

[2]*Department of Bioscience and Engineering, National Institute of Technology Calicut, NIT Campus PO, Kozhikode, 673601, Kerala, India*

*Corresponding author E-mail: sajith@nitc.ac.in

ABSTRACT

Marine biofouling remains a major challenge for the maritime industries, affecting both vessels and stationary installations. Various antifouling coatings are being utilized on ship hulls and structures to inhibit the growth of fouling organisms. This study investigates the use of MoS_2/Ag-TiO_2 (MAT) incorporated polyurethane coatings on mild steel as an effective antifouling coating. MAT nanocomposites were synthesized using liquid phase exfoliation process, and their structure and morphology were characterized using various spectroscopic and microscopic methods. The photocatalytic efficiency of the MAT nanocomposite was evaluated by measuring the degradation of crystal violet (CV) dye under sunlight, achieving an efficiency rate of 81 %. Antibacterial tests on *Staphylococcus aureus* (*SA*) and *Pseudomonas aeruginosa* (*PA*) revealed maximum photocatalytic killing activity at 600 µg/mL and 400 µg/mL, respectively. Furthermore, the utilization of MAT coatings in marine structures was investigated using a marine water consortium to assess their impact on inhibiting biofilm formation. The findings demonstrated a significant reduction (~ 95%) in bacterial adhesion compared to the uncoated surfaces, leading to a decrease in biofouling. Studies on microbial-induced corrosion demonstrate that MAT coatings display outstanding improvements in charge transfer resistance (4605 Ω) and coating resistance (7310 Ω). The toxicity assessment conducted on the MAT nanocomposite indicated an excellent biocompatibility with 94% cell survival at 400 µg/mL. This work demonstrates an environment-friendly and cost-effective anti-biofouling coatings employing the dual functionalities of photocatalysis and antibacterial properties of MAT heterojunction.

Keywords: Marine fouling coatings; Photocatalysis; Biofilm inhibition; Microbial induced corrosion; Environment-friendly coating.

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Enhancing Thermal Comfort and Energy Efficiency: Shape-Stabilized PCM Integration for Passive Cooling in RCC Roofs

Akshara A[1], Akbar Shanu[2], Sajith V[2] and Naseer M A[1,*]

[1]*Department of Architecture and Planning, National Institute of Technology Calicut,*

NIT Campus PO, Kozhikode,673601, Kerala, India

[2]*Department of Material Science and Engineering, National Institute of Technology Calicut,*

NIT Campus PO, Kozhikode,673601, Kerala, India

*Corresponding Author E-mail: naseer@nitc.ac.in

ABSTRACT

The construction industry significantly influences global energy usage, with heating, ventilation, and air conditioning (HVAC) systems representing over 60% of overall energy demand. Enhancing the thermal efficacy of building envelopes and systems offers a significant opportunity to reduce the energy use for indoor air conditioning. The incorporation of phase change materials (PCM) in building envelopes is an attractive option for the thermal management of buildings. PCMs store and release significant amounts of heat depending upon the ambient conditions. This study focuses on the development of a shape-stabilized PCM (SSPCM) for retrofitting reinforced cement concrete (RCC) roofs, aiming to enhance passive cooling efficiency. The shape-stabilized PCM was made by incorporating Lauric acid in Natural rubber, in various proportions. Experimental studies were carried out on the shape-stabilized PCM by measuring the transient temperature variation during heating. The simulation study was done on the SSPCM retrofitted reinforced cement concrete (RCC) roofs using Design Builder software to assess the thermal efficiency. Simulation results show that the integration of SSPCM in RCC roofs can reduce indoor temperatures by up to 3°C during peak temperature conditions, leading to improved energy savings and enhanced thermal comfort.
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Keywords: Phase changing materials; RCC roof retrofit; Passive cooling.

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Unearthing Low Overpotential of Platinum Electro-Grafted Ni-Co-S as Efficient Hydrogen Evolution Electrocatalyst

Arushi Arora* and Menaka Jha

Institute of Nano Science and Technology, Knowledge City, Sector 81, Mohali-140306

*Corresponding Author E-mail: arushi.ph20230@inst.ac.in

ABSTRACT

In the landscape of ever demanding sustainable energy sources, hydrogen stands as a beacon of hope, offering a clean and versatile escape to our pressing environmental challenges. The shift from fossil fuel-based fuels to the hydrogen economy has begun, as hydrogen possess an energy density of 120–140 MJ/kg, which is three times more energy-dense than petrol can offer. Water electrolysis tends to be cleaner alternative way to generate hydrogen in a sustainable manner. Designing efficient electrocatalysts for a sustainable and renewable energy conversion is crucial need of the hour. In this work rational use of Platinum, replacing the concept of "contaminating" to "activating" the base catalyst to maximally optimize the utilization of platinum for Hydrogen Evolution reaction (HER). Here, repeated linearly sweeping of potential is utilized to scavenge Platinum (Pt) on bimetallic sulphide material, Ni-Co-S nanoparticles supported on graphite strip. X-ray photoelectron spectra (XPS) give a clear proof of increasing deposition of Pt when cycled up to 2000 cycles. Transmission electron microscopy (TEM) mapping shows Pt particles deposited over spherical Ni-Co-S nanoparticles. The electro-grafted Pt on Ni-Co-Shas been used as excellent HER cathode with low overpotential of 48 mV ,high current density and a low value of R_{ct} of 58 Ω, in 0.5 M H_2SO_4 solution. The catalyst also shows excellent stability for HER for over 48 h. This practice serves as a facile method for synthesizing a non-hazardous and versatile electrocatalyst without involving any kind of elaborate treatment process.

Keywords: Hydrogen; Hydrogen evolution reaction (HER); Platinum; Water electrolysis.

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Experimental Investigation of Polyvinylpyrrolidone as an Artificial Synovial Fluid Material for Osteoarthritis Treatment

Sunil Anil More, Krishnadas Narayanan Nampoothiri
Department of Mechanical Engineering, Amrita School of Engineering, Amrita Vishwa Vidyapeetham, Chennai – 601103, Tamil Nadu, India
*Corresponding Author E-mail: sunilmore1009@gmail.com

ABSTRACT

Being a degenerative disease, Osteoarthritis need to be treated periodically to reduce the knee joint pain due to loss of joint lubrication which is termed as synovial fluid. For this purpose, efforts are being made to develop artificial synovial fluid. Till date, the most common fluid used is primarily based on hyaluronic acid. Even though the artificial synovial fluid offers temporary relief by enhancing joint lubrication, the treatment is expensive and has prolonged side effects post treatment. The main objective of this study is to develop an improved artificial synovial fluid that more closely mimics the rheological behaviour of natural human synovial fluid, offering a more effective and longer-lasting treatment for osteoarthritis. The initial study involves rheological testing of Polyvinylpyrrolidone (PVP) at different concentrations. PVP can be considered as biocompatible water-soluble polymer and has been effectively used as substitute in articular cartilages. Two distinct solvents (water and bovine serum) were used to create PVP40 solutions in five different concentrations (0-20 weight percent of PVP40). Rheological testing of the samples was performed on an Advanced Modular Rheometer. The rheological properties were measured in the low to higher shear rate range. It is observed that as the shear rate increases, shear stress is also increases for all the samples. Higher shear stress is observed for the 20% PVP with bovine serum as solvent. The samples displayed non-Newtonian shear thinning behaviour and the presence of bovine serum significantly modified the rheological properties of the sample. The present study proposed the viability of PVP as synovial mimic fluid and with the presence of bovine serum can improve lubrication properties.

Keywords: Synovial fluid; PVP; Bovine Serum; Knee joint; Osteoarthritis.

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Development of a Flexible Silicone Rubber-Silicon Carbide Heat Spreader for Low-Power Electronics

Akbar S, Arun K, and Sajith V*
Department of Materials Science and Engineering, National Institute of Technology, Calicut, NIT Campus PO, Kozhikode, 673601, Kerala, India
*Corresponding author E mail:: sajith@nitc.ac.in

ABSTRACT

Maintaining the temperature of electronic devices within the safe range is essential, as severe temperature can impair their performance. Heat spreaders are frequently used in electronic devices for effective thermal management and the low thermal conductivity of the heat spreaders is a challenge to be addressed. The present work focuses on developing a flexible heat spreader made of silicone rubber (SiR) incorporated with silicon carbide (SiC) particles. SiC was added in varying concentrations from 0 to 100 parts per hundred rubber (phr), and the mechanical and thermal properties of the composite were estimated. The concentration of SiC was optimised as 50 phr, as it exhibits optimal performance with favourable elongation at break, Young's modulus, and toughness, despite a slight reduction in tensile strength. Thermal conductivity and diffusivity were significantly enhanced by 266% and 277%, respectively, with the addition of SiC, and the 50-phr composite showed superior heat transfer as compared to pure SiR. Heat transfer studies were done on a smartphone with SiR-SiC composite heat spreader, by monitoring the transient temperature variation of the smartphone using infrared thermography. The results showed enhanced heat transfer performance as compared to pure SiR heat spreader, owing to the enhancement in the thermal conductivity of SiR. This research demonstrates the potential of SiR-SiC composites, for the next-generation thermal management of flexible, low-powered electronics, opening up new possibilities for wearable technology applications.

Keywords: Silicone rubber; Silicon carbide; Flexible heat spreaders; Low powered electronics.

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Comparative Analysis of Oil Residues: Material Characterization and Biodegradation Testing for Environmental Remediation as Frictional Concern

Sunil Kumar Hemanth M[1,*], J Edwin Raja Dhas[2]

[1]*Department of Mechanical Engineering,, Noorul Islam Centre for Higher Education, Kumaracoil, Kanniyakumari, India*

[2]*Department of Automobile Engineering,, Noorul Islam Centre for Higher Education, Kumaracoil, Kanniyakumari, India*

*Corresponding Author E-mail: m.sunil.k.hemanth@gmail.com

ABSTRACT

The automotive sector significantly contributes to global pollution, primarily through frictional interactions that generate tribological waste particles due to wear, fuel consumption, exhaust emissions, production processes, and end-of-life vehicle disposal. These particles can adversely impact air quality and public health while contributing to landfill waste, highlighting the urgent need for improved sustainability management in vehicle components. Biodegradation testing is crucial for the development and implementation of sustainable materials, ensuring that these materials can effectively decompose in the environment, comply with regulations, foster innovation, and meet the growing demand for eco-friendly products. This research explores the potential of oil residues as viable resource materials with frictional properties suitable for automotive applications. The study investigates Coconut Oil Residue (COR), Groundnut Oil Residue (GOR), Sesame Oil Residue (SOR), and a combination of all three (CGS) to assess their biodegradation characteristics. Each residue is inoculated with the bacterium *Acinetobacter baumannii*, commonly found in landfills and waste environments, to evaluate its life assessment from an eco-friendly perspective. Spectroscopic analyses, including Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray Spectroscopy (EDS), are employed to confirm elemental composition and conduct comparative analyses for environmental sustainability. The results demonstrate that these oil residues, particularly when combined with the bacterium, exhibit enhanced biodegradation properties, encouraging their implementation as friction materials in automotive components. This research highlights the potential of utilizing oil residues not only to mitigate environmental impact but also to innovate in the field of sustainable automotive materials.

Keywords: Oil residues; Biodegradation; Friction materials; Material characterization.

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Comparative Analysis of Fused-Crushed and Spray-Dried Mullite Powders for Atmospheric Plasma Sprayed Coatings

Syamkumar K[1,*], Narendra Babu[2], Shashi Bhushan Arya[2], Sumanth Govindarajan[2]

1: Department of Metallurgical and Materials Engineering, Amal Jyothi College of Engineering, Koovappally, Kottayam, India

2: Department of Metallurgical and materials Engineering, National Institute of Technology. Surathkal, Karnataka, India

*Corresponding Author E-mail: ksyamkumar@amaljyothi.ac.in

ABSTRACT

Two different morphologies of mullite powders-fused and crushed (FC) and spray dried (SD)-for atmospheric plasma spraying (APS) coatings. The FC coatings exhibited a surface morphology with larger splashed splats and significant open porosity (approximately 15%), while SD coatings demonstrated smaller, disc-shaped splats with a lower porosity of 4.41%. Despite the high mullite content in FC powder (98.4%), it dissociated more than SD powder, forming more metastable γ-Al_2O_3 phases in the APS coating. In-situ XRD tests revealed an increase in mullite and degradation of γ-Al_2O_3 in FC coatings upon heating. Differential Scanning Calorimetry (DSC) indicated a higher specific heat capacity for FC coatings, although they disintegrated at higher temperatures. Both FC and SD coatings exhibited comparable hardness; however, SD coatings, with approximately 23.5% secondary phases like α-Al_2O_3, showed a higher surface roughness. Interestingly, FC coatings demonstrated nearly double the thermal conductivity of SD coatings, attributable to more interfaces and improved thermal insulation due to distributed pores throughout the coating matrix.
Overall, characterizations revealed that SD powders are more suitable for plasma spraying than FC powders due to reduced dissociation and structural changes, offering superior mechanical and thermal properties post-deposition.

Keywords: Mullite; Thermal Barrier coating; APS; Material Characterisation.

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Piezoresistive Sensors from Pyrolyzed Coconut Fiber

Mohammed Mudassir [1], Ankur Verma[2], **Bushair Ali K**[3], Subash Cherumannil Karumuthil[2,*], C N Shyam Kumar[1,*]

[1] *Department of Materials Science and Engineering, National Institute of Technology Calicut.*

[2]*Centre for Nano and Soft Matter Sciences, Bengaluru*

[3]*Department of Physics, Sullamussalam Science College, Areekode*

*Corresponding Author Email: shyam@nitc.ac.in

ABSTRACT

Pyrolyzed carbon materials have garnered significant attention in recent years as a technologically relevant material, due to their interesting mechanical, electrical, and thermal properties. The locally available organic wastes such as coconut fiber can be pyrolyzed and tuned for their properties for various applications. The present study focuses on the fabrication of a piezoresistive tactile sensor from coconut fiber-derived carbon. Coconut fibre was pyrolyzed at 600°C (CCP600), 800°C (CCP800) and 1000°C (CCP1000) to produce a carbon material with promising electrical properties for sensor applications. From piezoresistive studies, it is evident that despite its lower conductivity (ρ = 1.342 Ωm, σ = 0.745 S/m), CCP-600 fiber demonstrates impressive piezoresistive characteristics, with a gauge factor (GF) of 29.8 ± 5.6. Alternatively, the gauge factor for CCP800 is 17.5 ± 3.2 and 5.2 ± 2.4 for CCP1000. With the increase in pyrolysis temperature, the gauge factor was reduced. The results for CCP600, CCP800 and CCP1000 also show varying resistance for different forces and weights measured. The resistance was measured at common voltages 0.5, 1, 1.5 and 2V. The results for different forces 0.3,3.9,6,8 and 11N show the highest variation up to 18kΩ for the CCP600, up to 173Ω for CCP800 and up to 50Ω CCP1000. The results for different weights 14.6, 58.3, 119.2 and 158.7gm show the highest variation up to 45kΩ for CCP600, 23Ω for CCP800 and 10Ω for CCP1000. This makes CCP600 well-suited for tactile sensors, where precise and reliable detection of mechanical pressure is crucial. CCP600, with its low cost and ease of fabrication, is a promising material for fabricating low-budget sensor applications.

Keywords: Pyrolyzed carbon; Coconut fiber derived carbon; Piezoresistive Sensors.

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Influence of Stacking Fault Energy on the Mechanical Behavior of Copper: A Molecular Dynamics Study

Aryan Soniya Duge[1,*], Punam Roy Suprio[1], Ebin P S[1], Karthik V Shankar[1] & Jeetu S Babu[2]

[1]*Department of Mechanical Engineering, Amrita Vishwa Vidyapeetham, Amritapuri, Clappana P O, Kollam – 690525, Kerala, India.*

[2]*Department of Materials Science and Engineering, National Institute of Technology Calicut, Kozhikode - 673601, Kerala, India.*

*Corresponding Author E-mail: aryan.duge@gmail.com

ABSTRACT

The stacking fault energy (SFE) is a key parameter that affects dislocation motion, deformation mechanisms, and the overall mechanical response of face-centered cubic (FCC) metals. This study investigates the influence of stacking faults on the mechanical properties of copper (Cu) using molecular dynamics (MD) simulations. In this work, the Embedded Atom Method (EAM) potential is employed to model the interactions in Cu, while a combination of tensile testing and the introduction of stacking faults allows for the simultaneous analysis of mechanical behavior and SFE. The results reveal a direct correlation between various parameters like stacking fault density, temperature, and system size, and changes in stacking fault energy, which subsequently influences the material's ductility, stress-strain response, and failure mechanisms. This study provides insights into the temperature and size dependent mechanical behavior of Cu, with potential implications for understanding deformation in other FCC metals.

Keywords: Molecular Dynamics; LAMMPS; Copper; Grain Stacking Fault Energy; Mechanical Properties.

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Tunable Dielectric Properties and EMI Shielding of MoS_2-Reinforced PVA/PEG Nanocomposites for Electric Vehicle Electronics Casings

Ankita Sarma[1], Aadil Jamshed[2], **Sudhanshu Nartam**[3], Anirban Sarkar[1], Nasirul Haque[2], Sandip Budhe[3], Jinu Paul[3]

[1]*Department of Physics, National Institute of Technology (NIT) Calicut, NIT Campus P.O., Kozhikode, Kerala, India 673601*

[2]*Department of Electrical Engineering, National Institute of Technology (NIT) Calicut, NIT Campus P.O., Kozhikode, Kerala, India 673601*

[3]*Department of Mechanical Engineering, National Institute of Technology (NIT) Calicut, NIT Campus P.O., Kozhikode, Kerala, India 673601*

*Corresponding Author E-mail: ankita_p230032ph@nitc.ac.in

ABSTRACT

The development of materials with both dielectric and electromagnetic interference (EMI) shielding properties is critical for electric vehicle (EV) applications, particularly for protecting sensitive electronics from high-voltage systems. In this study, PVA/PEG-blended nanocomposite films reinforced with MoS_2 nanosheets were synthesized via solution casting for EV battery casing requirements, including mechanical strength and EMI shielding properties. The incorporation of PEG into PVA reduced its crystallinity, leading to enhanced electrical conductivity. Furthermore, the PVA-PEG graft copolymer combined with conductive fillers such as MoS_2 significantly improved the dielectric characteristics. The dielectric constant of pure PVA was approximately ε = 16 at 20 Hz, whereas the PVA/PEG blend exhibited a dielectric constant of 33 at the same frequency. Nanocomposites with elevated MoS_2 loading (16 wt%) achieved a peak dielectric constant of 135 at 20 Hz. The structural properties of the PVA/PEG/MoS_2 composites were analyzed using Fourier transform infrared (FTIR) spectroscopy, revealing strong interactions between MoS_2 and the polymer matrix. Thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) confirmed improved thermal stability and variations in melting temperature with the addition of MoS_2. Furthermore, the EMI shielding effectiveness (SE) revealed that the composites achieved superior shielding effectiveness. This performance surpasses that of traditional aluminium materials, highlighting the potential of the composites for effective electromagnetic protection in EV battery casings and offering a lightweight, efficient, and safe alternative to conventional materials in the rapidly evolving electric vehicle industry.

Keywords: Polymer nanocomposite; MoS_2 nanosheets; dielectric properties; EMI shielding; electric vehicle

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Investigation on Mechanical Properties and Microstructure of Friction Stir Welded Aluminium AA1100 and Magnesium AZ31 Alloys for Lightweight Structural Applications

Binu Thomas*, P S Sreejith

Cochin University of Science and Technology,Kochi,India,682022

* Corresponding Author E-mail: binuthomas@cusat.ac.in

ABSTRACT

Multi-material lightweight structures are gaining a great deal of attention in several industries due to reduced weight, improved performances, and cost compression. To incorporate numerous light-weighting ideas in manufacturing, the replacement of steel or cast iron with light metals has been considered. Magnesium and Aluminium are two of the lightest structural metals and their alloys are finding increasing applications in industries mainly for their high strength to weight ratio. Aluminium and magnesium has a density of 2.7 g cm^{-3} and 1.74 g cm^{-3} respectively compared to steel density of 7.86 g cm^{-3}.However, there is usually unavailability of aluminium for high-volume production. Hence, the joining of aluminium to magnesium in the right proportion could be suitable for applications to mitigate the challenges faced with the usage of steel or cast iron and availability of aluminium and help to further reduce the weight and increasing its strength.The fabrication of such alloys is a challenging task through conventional fusion welding due to various metallurgical concerns. The objective of this work is to investigate the mechanical properties (tensile strength, hardness) and microstructure of friction stir welded (FSW) aluminium AA1100 alloy with most commercially available magnesium AZ31 alloys. The plates of 150x50x8 mm are joined by FSW using a non-consumable tool of probe size 5 mm made of maraging steel on a modified universal vertical milling machine. Defect-free weld was successfully obtained with a rotation speed of 600 rpm and feed rate of 5 mm/min.Various tests such as tensile test, hardness test, and microstructure analysis were conducted to evaluate the strength of the welded joint. The effect of tool probe size on tensile strength of the joint is also studied. From the results it was observed that the tool probe size shall be increased to get more penetration depth in order to increase the tensile strength of the joint at stir zone. Microstructural observations from optical microscope demonstrated that a complex vortex flow occurred in the stirred zone due to the intermetallic formation in the stir zone during the welding process. It was observed the formation of onion ring in the microstructure due to the presence of intermetallic compound (IMC) Al_3Mg_2 and $Al_{12}Mg_{17}$ from X-ray diffraction. The maximum value of hardness existing in the middle of the stir zone was twice higher than that of the base material due to the presence of hard IMCs. Combining AA 1100 and AZ31 alloys in one hybrid structure would make possible the use of these alloys for even more applications which will result in desirable weight saving without compromising its strength.

Keywords: Multi material; Maraging steel; Stir zone; IMC; X-ray diffraction.

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Experimental Investigation on the Effect of Process Parameters on Tensile Strength of Friction Stir-Welded Aluminium 8090 Alloys

Binu Thomas*, P S Sreejith

Cochin University of Science and Technology,Kochi,India,682022
* Corresponding Author E-mail: binuthomas@cusat.ac.in

ABSTRACT

The low density Al-Li alloy (8090 series) is a class of alloys with excellent strength and corrosion resistance that finds extensive use in the automotive and aircraft sectors. It is noteworthy that, in comparison to conventional aluminum alloys, adding Li (ρ of 0.53 g/cc) to aluminum alloy appears to reduce the weight structure by 10-15% and increase the stiffness to 15-20%.In precision industries, the fabrication of aluminum joints are challenging using traditional fusion welding due to the presence of segregation and porosities in the weld joint. Friction stir welding (FSW) has proven to be a dependable joining method to produce welds of high quality with no defects, reduced cost and lower environmental impact when compared to traditional fusion welding. One of the most important factors affecting heat generation, plastic flow, joint integrity, the resulting microstructure, and mechanical properties in FSW joint is the design of the tool, which includes material selection and shape. AISI H13 hot-worked tool steel has been found to be suitable for welding a variety of materials, because it has good machine ability and high level of abrasion resistance. The objective of this work is to identify the effect of process parameters on tensile strength of friction stir welded aluminium AA 8090 alloys and to optimize and validate the process parameters for maximum tensile strength. This study examined the effects of three controllable process parameters on tensile strength in FSW operation: tool rotating speed (800, 1000, 1200), weld speed (50, 70, 90), and shoulder to pin diameter (D/d) ratio (3, 3.5, 4). The studies were conducted on plates of 150x50x6mm of AA 8090 alloy on FSW 2T NC machine using H13 tool steel by applying the Taguchi technique. A three-level, three-factorial experimental design was created using Minitab 16 software, in accordance with the Taguchi L9 orthogonal array. The most significant factor and the percentage contribution of each individual factor to tensile strength were determined using the analysis of variance (ANOVA) and signal to noise (S/N) ratio. The results show that a rotational speed of 1200 rpm, a welding speed of 90 mm/rev, and a shoulder to pin diameter of 3 are the optimal values for tensile strength of friction stir welded AA 8090 alloys. The rotational speed is shown to be the most significant factor with a contribution of 68.6%.The second most important factor affecting the tensile strength is the ratio of the shoulder to pin diameter (D/d) followed by weld speed. It was also found that tool shoulder to pin diameter (D/d) ratio is critical in tool design for getting optimal results. Ultimately, a tensile strength value model derived from FSW parameters was computed and validated by testing outcomes. This analysis can be further used in predicting the empirical equations with which the process can be automated based on the optimal values.

Keywords: Al-Li alloy; D/d ratio; Taguchi L9 orthogonal array; ANOVA; S/N ratio.

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A Review on Anti-Bacterial Studies & In Silico Investigation of Lead Compounds from Selected Plant Extract

Aparna I*, Shahnaj N P, Fizza Nejmuddeen, Abhijith K S, Abhishek Das T, Haseena P V

Chemical Department, Government Engineering College Thrissur, Government Engineering College Thrissur P O, Thrissur, India.

*Corresponding Author E-mail: aparnakochumon049@gmail.com

ABSTRACT

The global spread of antibiotic-resistant bacteria can exacerbate health disparities between developed and developing countries. The increasing prevalence of antibiotic resistance puts an additional strain on the health care system resulting in economic losses. Lately, the search for natural alternatives to antibiotics is gaining momentum. Natural sources such as plants contain compounds with antibacterial properties that can be developed into new drugs. These natural compounds may have lesser side effects and potentially lower the risk of resistance. Recent studies have demonstrated the remarkable efficacy of plant extracts in inhibiting bacterial growth, with some exhibiting astonishingly potent antibacterial properties. In silico analysis have further identified lead compounds, showcasing strong binding affinities with bacterial target proteins. As the battle against antibiotic resistance intensifies, nature's armor may hold the key to unlocking novel solutions, and this review aims to inspire and galvanize researchers to harness the full potential of plant-derived compounds in the quest for new antibacterial agents.

Keywords : Plant extracts; Natural alternatives; Antibacterial properties.

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Piezoresistive Properties of Laser-Graphitized Polyimide Film for Low-Cost Flexible Sensor Applications

Krishnapriya U K[1], Arun V[2*], C N Shyam Kumar[2]

[1]*Department of Physics, PTM Govt College Perinthalmanna, Kerala, India*

[2]*Department of Material Science and Engineering, NIT Calicut, Kerala, India*

*Corresponding Author Email: arun_p230680mt@nitc.ac.in

ABSTRACT

Laser graphitization is a rapid and cost-effective technique for converting carbon-rich materials into graphitized carbon using high-power lasers. Unlike conventional furnace methods, laser graphitization is highly localized, eliminating the need to heat the entire substrate and can be performed in ambient conditions without a controlled atmosphere. In laser engraving modes, such as dot-filled engraving, parameters like dwell time, spot size, and fill interval significantly influence the precision and quality of the process. This study investigates the piezoresistive behaviour of laser-graphitized polyimide (Kapton) tape adhered to a polyethylene terephthalate (PET) substrate. The graphitization process was performed on four samples using a Snapmaker A350T machine equipped with a 10-watt laser module, with laser powers set to 16%, 18%, 20%, and 22%, respectively. Microstructural characterization was conducted using Raman spectroscopy and X-ray diffraction, revealing that the degree of graphitization increases with higher laser power. Piezoresistivity measurements using the two-probe method demonstrate that the sample treated at 16% laser power exhibits a higher gauge factor (10.498 ± 0.47) compared to those treated at higher powers. The enhanced piezoresistive performance at 16% makes it a promising material for sensing applications. Moreover, the use of a flexible substrate, combined with the ease of fabrication and low-cost production, underscores the potential of this material for low-budget sensor applications.

Keywords: Laser graphitization; Polyimide; Piezoresistive behaviour; Gauge factor; Flexible sensors.

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Electrospun PLA/Bioglass Nanofiber Coating on Mg-Ca Alloy for Tailored Biodegradation and Enhanced Bioactivity

Nithin S N, Aadil Shan, G Dhanyasakthie, Gokul Bhaskaran, VP Muhammad Rabeeh, T Hanas*

Applied Materials Research Laboratory, Department of Materials Science and Engineering, National Institute of Technology Calicut, Kozhikode, 673601, India

*Corresponding Author E-mail: hanas@nitc.ac.in

ABSTRACT

Magnesium (Mg) alloys are among the promising materials suited for biodegradable implant applications. However, the rapid degradation of Mg restricts its potential applications. Various surface and metallurgical modifications of Mg-based alloys are viable methods for tailoring their degradation rates. This study investigates the impact of electrospun polylactic acid/bio-glass composite (PLA/BG) nanofiber coating on the biodegradation, bioactivity, and biocompatibility of Mg-Ca alloy. The electrochemical corrosion measurement and *in vitro* degradation test were performed using biomimetic NaCl solution and simulated bodily fluid (SBF). The results indicated that the coated sample exhibited superior degradation resistance and bioactivity compared to the uncoated Mg-Ca alloy. It is observed that the hydrophilic PLA/BG coating enhanced biomineralisation and facilitated the *in-situ* formation of hydroxyapatite on the surfaces. The cell culture studies using L929 cells demonstrated that the coated samples are cytocompatible. Thus, it is concluded that PLA/BG electrospun nanofibrous coating is a viable approach to enhance biomineralisation and tailor the biodegradation of Mg-Ca alloy in the physiological environment.

Keywords: Mg alloy, Electrospinning; Polylactic acid, Bioglass; Biodegradation.

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Feasibility of Using Natural Fibres for Enhancing the Flexural Strength of Concrete

Gaurav Sancheti[1,*], Bhuvanesh Mathur[1], Shaik Hussain[2]

[1]*Department of Civil Engineering, Manipal University Jaipur, Dehmi Kalan, Jaipur, Rajasthan, India, 303007*

[2]*Research Scientist, Trenchless Technology Center, 1207 Agriculture Dr, Ruston, LA 71270, USA*

*Corresponding Author E-mail: gaurav.sancheti@jaipur.manipal.edu

ABSTRACT

Concrete is a hard mass formed by mixing raw materials such as cement, sand, aggregate and water. It gains strength with the elapse of time and in about 28 days, approx. 99% of its strength is achieved. Being very strong against compressive loads, concrete can merely (around 8 -10%) handle the flexural loads. Though there have been several studies with various types of proposed fibres for compensating flexural stresses, none have been standardised. This paper aims to sketch a review of the potential of natural fibres to be used in concrete. The types of natural fibres, their properties and the feasibility of using them in concrete are discussed. This review will support the engineering community in knowing the application criteria of various types of fibres and how these fibres may influence the strength characteristics of concrete.

Keywords: Concrete; Mechanical Strength; Flexural Strength; Fibre.

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Streaming Induced Hydrovoltaic Power Generation by Functionalized Graphene Derivatives

Neethu M, Sudip K Batabyal

Department of Physics, Amrita School of Physical Science, Amrita Vishwa Vidyapeetham, Coimbatore, India

*Corresponding Author E-mail: s_batabyal@cb.amrita.edu

ABSTRACT

The rapid growth of hydrovoltaic technologies by scavenging renewable energy sources for power generation provides a promising approach for self-powered devices. Out of recent literature, graphene-based materials with tunable properties were considered as a preferred choices to harvest electrical energy through hydrovoltaics due to their higher surface charge and porous nature. Here in this work, we are going to explore the electrokinetic studies of graphene-based derivative in both energy harvesting and energy storage sectors. The heterogeneous distribution of oxygen content along the highly oriented GO lamellae favors the less complicated ion (proton and hydronium ions in water) transport through the nanochannels. After the incorporation of most electronegative element Fluorine, hydrophilic GO became partially hydrophobic which results in the addition of surface functional group into GO lamellae. We fabricated a 3D hydrovoltaic power generator using fluorinated graphene oxide as an active material. Active material filled in a silicon ice tray with electrodes on top and bottom part and water will be dropped from top to bottom, which is different from conventional hydrovoltaic devices. We added ethylene glycol to generate a hydro-polymeric network to facilitate water movement. Using proton conducting polymer additives was found to be more effective for power generation by effectively releasing movable ions under moisture. When moisture comes into contact with fluorinated graphene oxide-polymer composite, protons and hydronium ions will ionize the surface functional groups and create a concentration gradient on the material-water interface. This concentration gradient will be generating a streaming potential which can able to results power generation. A droplet of water (20 µl) was poured on the top electrode, an open circuit voltage of 250 mV and a short circuit current of 100 µA with a power output of 625 µW/g. As time proceeds, potential difference started increasing and short circuit current decreases and gradually reach a steady state under ambient conditions. A single droplet can attain higher output and successfully power up low-power electronic devices. Addition of fluorine results in a comparable difference in the capacitance of bare graphene oxide and fluorinated graphene oxide. F could effectively provide a large number of active sites, showing a more prominent bilayer capacitance of 350 F/g and better cycling stability performance. It was found that the CV curves maintained a rectangular-like shape with no obvious distortion at both low and high scan rates, and the shape of the CV curves indicated that there was no redox reaction and the ion uptake process was dominated by the electric double-layer mechanism, and the electrolyte migration channels were increased by the establishment of the nanoporous structure with the help of fluorine.

Keywords: Sustainable development; Renewable energy sources; Hydrovoltaic power generation; Streaming potential; Electric double layer.

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Molecular Dynamics Study of the Latent Heat of Nano-Enhanced Phase Change Materials

Gokul M Pillai[1], **Madhu A K[2,*]**, C B Sobhan[3]

[1] *Department of Mechanical Engineering, Indian Institute of Technology, Indore, India*

[2]*Dept. of Mechanical Engineering, College of Engineering Adoor, India*

[3]*Department of Materials Science and Engineering, NIT Calicut, India*

*Corresponding Author E-mail: madhuak@cea.ac.in

ABSTRACT

Phase change materials (PCM) serve as effective media for thermal energy storage. To enhance the thermal conductivity of these materials, nanoparticles are often incorporated. However, the majority of existing research has primarily concentrated on the improvement of thermal conductivity, often overlooking the consequent reduction in latent heat of the PCM associated with the addition of nanoparticles. The present study utilizes equilibrium molecular dynamics simulations within a computational framework featuring graphene sheets suspended in water, to investigate the mechanisms that may lead to a reduction in the latent heat of fusion of ice when graphene sheets are introduced. The findings reveal a notable decrease in the latent heat of ice with the addition of 0.5 wt% graphene. Moreover, the addition of graphene also causes a significant drop in the melting temperature of the ice. Additionally, the results indicate that the presence of graphene sheet accelerates the melting process. Analysis of the radial distribution function confirms the occurrence of phase transition within the system. Simulations also point to the formation of strong interfacial layering around the graphene sheet. The presence of this layering is identified as a key factor contributing to the observed reduction of the latent heat of fusion of the nano-enhanced phase change material.

Keywords: Latent heat; Phase change material; Equilibrium molecular dynamics; Nanoparticle.

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Investigating the Feasibility of Green Nanoparticle Synthesis for Detecting Adulteration in Honey

Vidya T P[1,2,*], Liza James[1], Saritha K Nair[1]

[1]*Department of Physics, Mar Athanasius College (Autonomous) Kothamangalam, India*

[2]*Department of Science and Humanities, Federal Institute of Science and Technology, Angamaly, India*

*Corresponding Author E-mail: vidyatp@fisat.ac.in

ABSTRACT

Honey, a highly valued natural food product, is often subject to adulteration, particularly with sugar syrups, posing challenges for quality assurance. While metal nanoparticle synthesis using honey as a reducing and capping agent has been previously reported, this study explores a novel approach to detecting honey adulteration via the green synthesis of silver nanoparticles. In this preliminary investigation, silver nanoparticles were synthesized through a sunlight-induced, honey mediated process using both pure and adulterated honey samples, with silver nitrate serving as the silver ion source. Notable differences in the optical properties, such as a marked decrease in the surface plasmon resonance (SPR) peak and absorbance values, were observed with adulterated samples, suggesting reduced efficacy in nanoparticle synthesis. This method, which requires minimal expertise and small sample quantities, offers a simple, environmentally friendly, and cost-effective approach that could complement existing techniques in food quality assessment. High-resolution transmission electron microscopy (HR-TEM) along with selected area electron diffraction (SAED) confirmed the formation of nanoparticles, while variations in surface plasmon peaks and refractive index values suggest the potential of this method to distinguish between pure and adulterated honey samples. While further studies are needed to enhance efficacy comparison, these findings highlight green synthesis of silver nanoparticles as a feasible tool in food quality assurance, with possible applications extending to other foods.

Keywords: Green synthesis; Honey adulteration detection; Food quality assessment; Metal nanoparticles.

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Green Synthesis of NiO Nanoparticles Using Waste Tea Extract and Their Utilization as Potential Electro-Anode for Ethanol Oxidation

Kritika Sood[1,2], Arushi Arora[1], K K Bhasin[2], Menaka Jha[1*]

[1]*Institute of Nano Science and Technology, Knowledge City, Sector-81, Mohali, India*

[2]*Department of Chemistry, Punjab University, Sector-14, Chandigarh, India*

Corresponding Author E-mail: menaka@inst.ac.in

ABSTRACT

This study presents a novel approach, aimed at developing sustainable energy material. Green synthesis of nickel oxide (NiO) nanoparticles was done using waste tea extract. The synthesized NiO nanoparticles were tested for electro-oxidation of ethanol, demonstrating a notable reduction in overpotential from at 0.44 V (in 1 M KOH + 1 M ethanol) from 0.67 V (in 1 M KOH) at a current density of 10 mA/cm². Comparative analysis with a benchmark platinum-based electrocatalyst revealed that the green NiO-NPs exhibited superior intrinsic kinetics and mechanistic performance, with a lower Tafel slope of 102 mV/dec and an electrochemical impedance spectroscopy (EIS) resistance of 26 Ohms. These results underline the efficiency and economic viability of using a bio-inspired method for synthesizing NiO nanoparticles, while also stressing the potential for upcycling waste tea. This innovative approach offers significant implications for the development of eco-friendly and sustainable energy conversion technologies.

Keywords: Green synthesis; NiO nanoparticles; Electrocatalysis; Advanced oxidation process; Ethanol oxidation.

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Effect of Dual Excitation on Tamm Plasmon Polariton Mode

Naseeb Abdu Taikkaden, Anirban Sarkar*

Department of Physics, National Institute of Technology Calicut, Kozhikode – 673 601, Kerala, India

*Corresponding Author E-mail: anirban@nitc.ac.in

ABSTRACT

Plasmonics based nanophotonics is a fascinating area of research due to its potential to provide high-end future ready optoelectronic technologies. Surface plasmon polariton (SPP) plays a major role in the plasmonic based nanophotonic devices. SPP is a mode of electromagnetic (EM) wave localized at a metal-dielectric interface [1]. When the metal layer is coated on a distributed Bragg reflector (DBR), the localized mode excited at the metal-DBR interface, is known as Tamm plasmon polariton (TPP) [2]. Unlike the SPP, which can be excited only by indirect techniques such as prism or grating coupling, TPP can be excited by direct interaction of EM waves with a dielectric structure. In the recent past, TPP has been studied extensively due to its wide range of applications in sensors, lasers, perfect absorbers and hot-electron photodetectors [3]. However, a detailed investigation on different excitation schemes of TPP mode has not yet been explored. Here, we investigate the TPP in a silver-DBR structure for single side and both side excitations and compare the field confinement under these excitation schemes. The numerical simulation is performed using COMSOL Multiphysics software. The structure consists of a DBR and a 50 nm thick silver film on the top of it, where the number of DBR bi-layers is varied. The EM wave of power $P_{inc} = 1$W in the optical frequency range is used for exciting the structure. The reflectivity of the structure is studied for different numbers of DBR bi-layers by exciting it from the silver side and as well as the DBR side. We observe that the metal side excitation is more efficient for better confinement of the TPP mode. Further investigation by splitting the same excitation intensity into two parts ($P_1 = 0.5$W and $P_2 = 0.5$W) for both side excitation shows enhanced field confinement of the TPP mode compared to that of the single side excitation as shown in Fig. 1. This enhancement is achieved by controlling the respective phases of the excitation waves. These results would be useful for developing novel optoelectronic devices utilising different excitation schemes of the TPP modes.

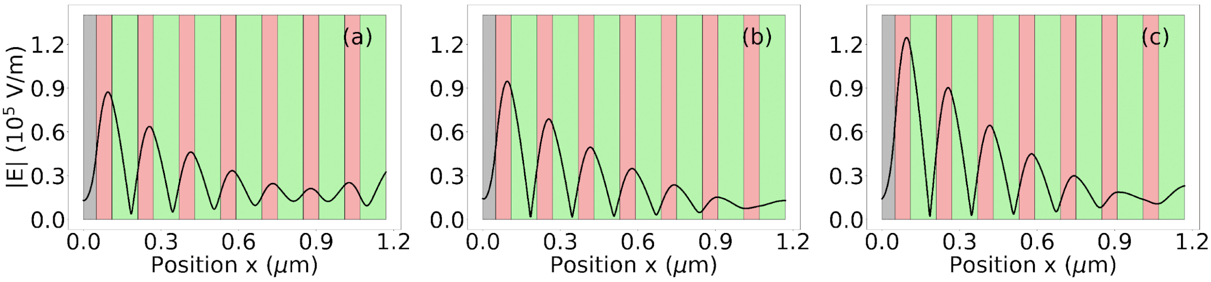

Fig. 1: The electric field distributions (shown in black line) inside the silver-DBR structure with Ag (grey) on the DBR structure made up of TiO_2 (red) and SiO_2 (green) for (a) DBR

side excitation, (b) metal side excitation and (c) both side excitation.

Keywords: Tamm plasmon polariton; Distributed Bragg reflector; Dual excitation; Optoelectronic devices.

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Effect of Montmorillonite Nano-Clay on the Flexural Behaviour Ti6Al4V Titanium-Based Carbon Fibre/Epoxy Laminates: An Experimental Investigation

Mohammed Jamsheed[1], Faizan Mohammad Rashid[1,*], R. Velmurugan[2]

[1]*Dept. of Mechanical Engg, Birla Institute of Technology and Sciences Pilani, Rajasthan, India.*
[2]*Dept. of Aerospace Engg, Indian Institute of Technology Madras, Chennai, India*
*Corresponding Author E-mail: faizan.rashid@pilani.bits-pilani.ac.in

ABSTRACT

A detailed experimental investigation was carried out to investigate the role of montmorillonite (MMT) nano-clay on the flexural properties of the Ti6Al4V titanium-based carbon fibre/epoxy laminates. Flexural tests were carried out as per ASTM D790 standard on a Kalpak Universal testing machine fitted with a 20kN load cell with crosshead speed maintained at 2mm/min. The test samples were cut into sizes of 120mm in length and 13mm in width, keeping the span-to-depth ratio of 16:1. The nano-clay reinforcement affected the flexural stress-strain behaviour of the Ti6Al4V titanium-based carbon fibre/epoxy laminates. FMLs, without any nano-clay reinforcement, were considered the baseline for comparison of the flexural properties of other nano-clay-reinforced FMLs. The flexural stiffness showed appreciable improvement for a higher weight percentage of nano-clay in the epoxy. Among the nano-clay reinforced FMLs, there was a clear improvement in the strength and stiffness with an increase in the weight percentage of the nano-clay; however, with some reservations. There was a fall of 49.92% and 50.53% in flexural strength and stiffness, respectively, with 1% of nano-clay addition into the epoxy. The dominant agglomeration phenomena played an essential role in lowering flexural strength and stiffness. Interestingly, an increase in the weight percentage of nano-clay led to an improvement in adhesion between titanium and the composite layer, and the phenomenon of mechanical locking started operating, which can be seen as an immediate improvement in the flexural strength for 3, 5 and 7% nano-clay reinforcement. The flexural stiffness also improved for 3 and 7% nano-clay reinforcement, with a fall of 17.85% for 5% nano-clay reinforcement. There was a fall in flexural strength and a rise in flexural stiffness for 5% nano-clay reinforcement. The phenomena of crack bridging also play a role in affecting flexural strength and stiffness.

Keywords: Fibre metal laminate; Titanium alloy; Carbon fibre; Flexural strength; Flexural stiffness.

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Effect of Montmorillonite Nano-Clay on the Mechanical and Thermal Properties of Pla-Based 3D-Printed Honeycomb Structures

Muzammil Ahmed Khan[1], Faizan Mohammad Rashid[1,*], Ngoc San Ha[2]

[1]*Dept. of Mechanical Engg, Birla Institute of Technology and Sciences Pilani, Rajasthan, India.*
[2]*Center for Innovative Structures and Materials, School of Engineering, RMIT University, Australia*
*Corresponding Author E-mail: faizan.rashid@pilani.bits-pilani.ac.in

ABSTRACT

Additive manufacturing, commonly known as 3D printing technology, has revolutionized the creation of complex architectures, including bioinspired structures. These structures are often topologically optimized, balancing lightweight design, high strength, and toughness properties characteristic of many biological materials. The 3D manufacture of complex multifunctional material systems with adjustable optical, chemical, and mechanical characteristics is made possible by 3D photo polymerization-based techniques. The present work explores the effects of montmorillonite nano-clay (MMT) reinforcement on Polylactic acid's mechanical and thermal properties, commonly known as PLA-based 3D-printed honeycomb structures with varying concentrations of MMT. Including M1 (pure PLA resin), M2 (PLA resin with 1% MMT), M3 (PLA resin with 3% MMT), and M4 (PLA resin with 5 % MMT). Dispersion techniques using magnetic stirring were used to disperse nanoparticles. A Prusa SL1S stereo lithography apparatus (SLA) was used to print honeycomb panels. Printed specimens were subjected to the tensile, bending and compression tests. Scanning Electron Microscopy, Energy Dispersive Spectroscopy, X-ray Diffraction, Thermal Gravimetric Analysis, and Fourier Transform Infrared Spectroscopy were used for characterization study. A correlation was developed between these performance parameters and the weight percentage of the nanoparticles. The SEM and EDX analysis revealed remarkable properties, such as a surface structure devoid of fractures, pores, and cavities and substantial carbon stretching in almost all samples obtained by FTIR. TGA results showed that under heating conditions, how samples had essentially the same characteristics and showed essential signs of crystallization in XRD analysis.

Keywords: 3D SLA printing; Nanocomposite; TGA; XRD; FE-SEM.

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Coconut Shell Derived Pyrolyzed Carbon for EMI Shielding

Haleema Safa[1], Mohammed Mudassir[2], Pisharody Harikrishnan G[3],

Nikhil Kumar C S[4], C N Shyam Kumar[2,*]

[1]*Department of Physics, Kannur University, Kannur, Kerala, India*

[2]*Department of Materials Science and Engineering, National Institute of Technology Calicut, Kerala, India*

[3]*Department of Electrical Engineering, Indian Institute of Technology Palakkad, Kerala, India*

[4]*Department of Electronics and Communication Engineering, National Institute of Technology Calicut, Kerala, India*

*Corresponding Author E-mail: shyam@nitc.ac.in

ABSTRACT

Pyrolysis of locally available organic wastes is trending in current research. Pyrolyzed carbon materials derived from these organic wastes have shown promising results to be used in wide variety of applications such as electromagnetic interference shielding. A detailed study of the structural and property evolution during pyrolysis is necessary to use these materials effectively. In this work, the structural evolution of coconut shell derived carbon is studied using XRD, Raman spectroscopy and scanning electron microscopy. Furthermore, the evolution of EMI shielding effectiveness of pyrolyzed carbon derived from coconut shell is studied. Coconut shells are subjected to pyrolysis at different high temperatures 600°C (CSP600), 1000°C (CSP1000) to produce pyrolyzed carbon. The morphology studies using SEM confirms the evolution of the porosity. The structural evolution is studied using Raman spectroscopy and XRD confirms the ordering and growth of sp^2 graphitic domains. Vector network analyser (VNA) is used for finding EMI shielding efficiency. Preliminary result indicates that the coconut shell-derived carbon exhibits a promising shielding effectiveness above 15dB, with a significant absorption and reflection of electromagnetic waves in the 8-12GHz frequency range. Recent study suggests that the coconut shell derived carbon can be used as a sustainable and cost-effective material for EMI shielding applications. These bio-based materials like pyrolyzed carbon from coconut shells can offer an eco-friendly alternative to conventional synthetic materials, contributing to sustainable development in EMI shielding technologies.

Keywords: Pyrolyzed carbon; Coconut shell; Electromagnetic Shielding.

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Development of a Portable Non-Enzymatic Paper Field Effect Transistor-Based (PFET) Sensor for Wearable Sweat-Glucose Monitoring Applications

Ayshathil Bushra K*, Sudhakara Prasad K
[1] *Nanomaterial Research Laboratory (NMRL), Smart Materials and Devices, Yenepoya Research Centre, Yenepoya University, Deralakatte, Mangalore 575 018, India.*
*Corresponding Author E-mail: ayshmangalore@gmail.com

ABSTRACT

Diabetes is a growing global health challenge, necessitating the development of affordable and reliable glucose monitoring technologies. Here, the semiconducting silver (Ag) nanoparticle (NP) decorated cuprous oxide (Cu_2O) dispersed on reduced graphene oxide (rGO) was synthesized by a rapid, cheaper microwave-assisted method. The material characterization techniques confirm the formation of nanocomposites (NC), patterned as the transistor sensing channel material. The charge (cation/anion) generated by the electrolytes (analyte) and NC interaction develops interface potential and electric double layer (EDL)/ capacitance change that stimulates channel conductivity. The faster electron and hole mobility, coupled with the superior selectivity of Ag-Cu_2O and the high conductivity of rGO, collectively contribute to excellent electrocatalytic activity for glucose oxidation. The fabricated PFET sensor could achieve a limit of detection (LOD) of 96 µM with high sensitivity and self-amplification effect. Real-time applications using artificial sweat introduced with a physiological range of sweat glucose concentrations (0.01 mM - 0.1 mM) yielded promising findings. Integrating the sustainable PFET chip with the electronic circuit improves comfort and usability, making it a practical choice for point-of-care (POC), wearable, and continuous glucose monitoring.

Keywords: PFET Chip; Sweat Glucose Sensor; POC Device; Wearable Sensor.

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Preparation and Characterization of a Novel Organic-Inorganic Eutectic Phase Change Material for Medium-Temperature Applications

Falgun Raval, Ruben Sudhakar D*

Department of Energy and Environment, National Institute of Technology Tiruchirappalli, Tamilnadu, India

*Corresponding Author E-mail: rubensudhakar@nitt.edu

ABSTRACT

Latent heat storage using phase change materials is among the promising solutions to bridge the gap between mismatched thermal energy supply and demand. This paper presents the preparation and characterization of a novel organic-inorganic eutectic phase change material (PCM) composed of Myo-inositol and Lithium Nitrate, designed for medium-temperature thermal energy storage applications. The preparation of the eutectic mixture was achieved using an indirect mixing method, and varying compositions were prepared with 10 wt.% mass ratio variations. Differential Scanning Calorimetry (DSC) analysis identified the ideal eutectic composition as 72:28 (wt.%) Myo-inositol:$LiNO_3$ with a melting onset of 196°C and the crystallization getting triggered around 149.9°C. The latent heat of fusion is found to be 148.63 kJ/kg, and the material subjected to 2 charge-discharge cycles shows good repeatability in terms of the melting point while only losing around 25 kJ/kg of latent heat, which can be attributed to the initial cycle's water vapor mass loss from the material. The thermal properties of this composition were further evaluated through Thermogravimetric Analysis (TGA) under an inert nitrogen atmosphere. The material exhibited excellent thermal stability for temperatures exceeding 275°C, with the onset of significant mass loss recorded at 295.18°C, indicating suitability for medium-temperature applications. The chemical stability of the eutectic PCM was assessed using Fourier Transform Infrared Spectroscopy (FTIR), which confirmed that no new functional groups were introduced during the formation of the eutectic, thus ensuring that the reaction was purely physical in nature and that the base materials didn't chemically react with each other. These results demonstrate that the prepared eutectic PCM holds potential as an efficient and thermally stable material for medium-temperature applications, such as in energy storage systems, where it can contribute to enhancing energy efficiency and sustainability.

Keywords: Phase Change Material; Organic-Inorganic Eutectic; Medium temperature thermal energy storage.

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A Portable Handheld Multimodal Spectroscopic Probe System for Monitoring the Quality of Coconut Oil

Liza James[1,*], Malavika Ramesh[2], Anusree Ajay[2], Shinoj V K[2], Saritha K Nair[1]

[1]*Department of Physics, Mar Athanasius College (Autonomous), Kothamangalam, Kerala, India*
[2]*Department of Physics, Union Christian College, Aluva, Kerala, India*
*Corresponding Author E-mail: lizajamesvm@gmail.com

ABSTRACT

Oil adulteration has a profound impact on both consumer health and market integrity. Paraffin oil is a common adulterant in coconut oil, as it is low-cost, readily available, colorless, tasteless, and odorless. This study examines coconut oil adulterated with paraffin oil. The absorbance spectra of pure and adulterated oils were measured with a portable, custom-built spectrometer (Rev. Sci. Instrum. 91, 073104, 2020) and compared and a notable decrease in the absorbance values below 450 nm was observed. This study demonstrates the applicability of the portable, custom-built spectroscopic probe as an instrument for detecting food adulteration. This handheld, portable, multimodal fibre optic based probe scheme will enable real time in-situ analysis making quality assessment accessible at any point; highlighting the multifunctionality of the probe. The FTIR spectra of the samples were also compared as a complementary measurement. Color measurements of the samples are underway, and the parameters extracted will be compared to assess the effectiveness of this tool in detecting adulteration.

Keywords: Oil Adulteration; Portable spectroscopic probe; FTIR spectroscopy; Color Measurement; Food Quality Assessment.

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Effect of Curcumin on Electrospinnability of Different Concentrations of Polyvinyl Alcohol Nanofibrous Scaffolds for Wound Healing Applications

Lamiya Nasreena, Nithin S N, Hanas T*

Applied Materials Research Laboratory, Department of Materials Science and Engineering,

National Institute of Technology Calicut, Kozhikode - 673601

*Corresponding Author Email: hanas@nitc.ac.in

ABSTRACT

Incorporating curcumin in biocompatible electrospun polymeric membrane can fetch numerous applications in the biomedical field, especially in wound healing. However, the incorporation of dispersed phase in a polymer affects formation of fibres during electrospinning. This study investigates the effect of curcumin concentration on electrospinning of polyvinyl alcohol (PVA) nanofibrous scaffolds. Powdered curcumin samples are incorporated into PVA solution at varying concentrations of 5 mg, 10 mg, 20 mg, 30 mg, 40 mg and 50 mg into o10 ml of PVA solution. PVA solutions with different viscosity was prepared by dissolving 0.6 g, 0.7 g, 0.8 g, 0.9 g and 1 g of PVA in 3:1 deionized water - ethanol solvent. The electrospinning process parameters such as voltage, feed rate, and tip to target distance were systematically varied to evaluate the influence of curcumin on the electrospinning and morphology of the PVA nanofibers. Scanning electron microscopy and optical microscopy confirmed that 10% PVA and 5 mg curcumin combination given a good extracellular membrane architecture. It is seen that fine tuning the electrospinning parameter can help incorporation of curcumin in the PVA electrospun membrane that can be used for would healing applications.

Keywords: Polyvinyl Alcohol; Wound healing; Curcumin; Electrospinning; Nanofiber

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Anodized Aluminium-Graphene Nanocomposite Heat Spreaders for Enhancing Heat Dissipation from Lithium-Ion Batteries

Shijina S S[1,2], Akbar S[2], Sajith V[2,*]

[1]*Department of Chemical Engineering, TKM College of Engineering, Kollam*

[2]*Department of Materials Science and Engineering, NIT Calicut*

*Corresponding Author E-mail: sajith@nitc.ac.in

ABSTRACT

Aluminium heat spreaders are used in battery packs of electric vehicles for enhancing the heat dissipation. The present work focuses on the development of anodized aluminium-graphene with enhanced heat dissipative properties for controlling the hot spot formation in battery packs. Powder metallurgy was adopted for the fabrication of aluminium (A) and aluminium -graphene composite (AG) heat spreaders. A 20% enhancement in the thermal conductivity was achieved with the addition of 0.5 wt.% of few-layered graphene for the composite heat spreader as compared to the plain aluminium heat spreader. Anodisation of the AG heat spreader yielded a thin layer of aluminium oxide on the surface and the surface roughness was found to be 40 times more than the non-anodized plain aluminium sample. Also, the presence of an anodized aluminium oxide layer has improved the surface emissivity to ~0.7 whereas for plain aluminium it is only 0.1. The synergistic effect of thermal conductivity, surface roughness/area and emissivity results in a faster heat dissipation in the composite heat spreader.

Keywords: Electric vehicle; Thermal management; graphene; Aluminium; Powder metallurgy.

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Highly Active Nickel and Nitrogen-Doped Carbon for Enhanced Water-Splitting Reactions

P A Junaid[1], S Sriram[1], K giddaerappa[1], K Sudhakara Prasad[1,2]*

[1]*Nanomaterial Research Laboratory, Smart Materials And Devices, Yenepoya (Deemed to be University), Deralakatte, Mangalore - 575 018, India*

[2]*Centre for Nutrition Studies, Yenepoya (Deemed to be University), Deralakatte, Mangalore - 575 018, India*

*Corresponding Author E-mail: ksprasadnair@yenepoya.edu.in

ABSTRACT

Developing earth-abundant and less expensive catalysts with high activity for water splitting is necessary to meet sustainable hydrogen production among the promising alternatives to precious metal catalysts. Nickel and nitrogen-doped carbon present high catalytic activity, stability, and cost-effectiveness. Ni–N–C catalysts were synthesized and assessed for their performance in alkaline (KOH) conditions in both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Along with the synthesized material, graphene oxide was incorporated into the material. The materials' structure can be considered a reason for efficient electron transfer and better catalytic activity due to uniform nickel sites and nitrogen-rich carbon matrix. Such overpotentials for water-splitting are diminished by the synergistic effect between the nickel and nitrogen sites in the carbon matrix, which thus reduces the energy demand for this splitting process. Electrochemical tests have exhibited that these Ni–N–C catalysts reveal remarkable stability and activity compared to Noble metal-based catalysts. It indicates the perspective of these Ni–N–C materials as scalable and economical catalysts, which can render practicality to water-splitting applications in this research study to accelerate renewable hydrogen production technology development. Secondly, wastewater deals with the deficit of fresh water; it dilutes wastewater into better and more sustainable energy.

Keywords: Electrochemistry; Water Splitting; Hydrogen Evolution Reaction (HER); Oxygen Evolution Reaction; Nickel; Nitrogen and Carbon.

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Development of Disposable Electrochemical Sensor as a Point-of-Care Testing Platform for Deficiency of Vitamin D

Inchara R K., Sudhakara Prasad*

Nanomaterial Research Laboratory, Smart Materials And Devices, Yenepoya (Deemed to be University), Deralakatte, Mangalore 575 018, India

*Corresponding Author E-mail: ksprasadnair@yenepoya.edu.in

ABSTRACT

The major source of vitamin D for most humans is exposure to sunlight. Around 1 billion people worldwide have vitamin D deficiency. Vitamin D deficiency is reported as a global health concern. Long-term deficiencies in this vitamin have been linked to blood clotting issues, diabetes, cancer, rheumatoid arthritis, osteoporosis and thus its detection must be accurate. Clinically speaking, serum 25(OH)D3 is regarded as one of the most exceptional biomarkers for the precise measurement of vitamin D levels. This study presents the novel electrochemical sensor for the quantification of vitamin D levels with high precision. The immunosensor was constructed by fabricating electrochemical paper analytical devices (e-PAD). The e-PAD utilises the versatile graphitic carbon nitride as an electrochemically active platform for the establishment of a sandwich immunosensor. Different electroanalytical techniques are used to analyse sensor performance and also analytical parameters are studied by recording recovery studies, spike sample and real sample analysis. The results are found to be quite indicative with a clear correlation between concentration and electrochemical response of vitamin D; thus, it can be applied for sensitive and cost-effective rapid diagnosis of vitamin D deficiency.

Keywords: Vitamin D; Electrochemical paper analytical devices (e-PAD); Serum 25(OH)D3; Graphitic carbon nitride; Sandwich immunosensor.

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Enhancing Sustainable Recycling of Aluminum Scrap through Advanced Alloy Development

Navin V Varughese[1], Athul Krishna P B[2], Adhi Ganesh[2], Emil Eldho [2], Meera Marium Toms[2], Arun Lalachan[2], Anoop K Unni[2], Mebin T Kuruvila[2, *]

[1]*Department of Metallurgical Engineering, Amal Jyothi College of Engineering, Kanjirappally, Kerala, India*

[2]*Department of Materials Engineering, Amal Jyothi College of Engineering, Kanjirappally, Kerala, India*

*Corresponding Author E-mail: mebintkuruvila@amaljyothi.ac.in

ABSTRACT

This research focuses on enhancing the mechanical properties of recycled aluminum 6063 scrap with the aim to reduce waste and promote sustainability. While conventional recycling typically results in substantial compositional and property losses, aluminum scrap especially from the construction and automotive industries offers significant opportunities for strong, sustainable and high-performance uses. The objective of this work is to increase the applicability of recycled aluminum as a metal matrix composites for demanding applications employing casting process. For this, aluminum 6063 scrap primarily sourced from automotive and construction structures were collected and melted in a muffle furnace. The study involved incorporating two different reinforcements namely silicon carbide (SiC) and boron carbide (B_4C) into the molten aluminum scrap matrix to make the ingot. In order to examine the distribution and influence of reinforcements on grain structure, microstructural analysis using optical microscopy and SEM analysis were performed. Mechanical properties were evaluated through tensile testing, Vickers microhardness, and wear testing on both reinforced and unreinforced samples. Both reinforcements were found uniformly distributed with B_4C showing finer grain refinement. Mechanical tests indicated that B_4C reinforcement performed significantly better than SiC. Thus, the study demonstrates that with recycling, waste can be decreased while material properties are greatly improved, establishing recycled aluminum 6063 metal matrix composite as a sustainable substitute.

Keywords: Aluminium 6063; High performance alloy; Metal matrix composites; Sustainability; Tensile strength.

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Chemical Kinetic and Thermodynamic Effects of Activating Flux Powders on TIG Weld Penetration in 304 L Stainless Steel

Anu Joy [1], Shreya P [1], Edwin Koshy Thomas[1], Arshad V Khader[1], Aleena George[1], Alex Biju[1], Mohammed Izzuddeen[1], Radhika S[2], Anoop K Unni[2, *]

[1] *Department of Chemical Engineering, Amal Jyothi College of Engineering, Kanjirappally, Kerala, 686518, India.*

[2]*Department of Metallurgical and Materials Engineering, Amal Jyothi College of Engineering, Kanjirappally, Kerala, 686518, India*

*Corresponding Author E-mail: anoopkunni@amaljyothi.ac.in

ABSTRACT

The use of activating flux powders in TIG welding of stainless steel has been found to enhance penetration depth, leading to stronger welds. These fluxes promote kinetic effects by accelerating chemical reactions at the weld interface, thereby increasing the rate of metal melting and fusion. Thermodynamically, the fluxes reduce the Gibbs free energy of the system, making the welding process more energetically favorable and efficient. This dual effect of improved kinetics and thermodynamics ensures better weld quality and productivity, making activating flux powders a valuable addition to TIG welding processes for stainless steel. In this study, five different combinations of oxide-based flux powders were employed namely NiO, CO_3O_4, V_2O_5, Cr_2O_3 and TiO_2. The activated- TIG welding experiments were conducted including one without any flux. By adjusting the oxide flux components, varying levels of dissolved oxygen were introduced into the weld pool, leading to differences in weld pool characteristics. To examine the chemical reactions involved between the fluxes and weld pool, XRD analysis of weld slag and thermodynamic calculations of Gibbs free energy changes were analyzed. Findings reveal that the type of chemical reaction between the flux and weld pool metal plays a crucial role on arc constriction.

Keywords: Activated-TIG welding; Chemical kinetics; Gibbs Free energy; 304L SS; Weld pool.

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Enhanced Seawater Electrolysis for Hydrogen Production Using a Nickel Ferrate/Nickel Oxide Catalyst Supported on Nitrogen-Doped Carbon

Sundarraj Sriram[1], Abdul Junaid[2], Giddaerappa[2], and K Sudhakara Prasad[2]*
Nanomaterial research laboratory (NMRL), Nano Division, Yenepoya Research Centre, Yenepoya (Deemed to be University), Deralakatte, Mangalore 575 018, India.

*Corresponding Author E-mail: ksprasadnair@yenepoya.edu.in

ABSTRACT

Hydrogen production from the electrolysis of seawater is more attractive than that from pure water, especially in regions where freshwater resources are scarce. However, under such harsh conditions, higher requirements are put forward for the catalytic activity and adaptability of a catalytic electrode. Herein, we synthesize affordable and highly active nickel-iron oxide fused with nitrogen doped carbon by simple pyrolysis method for an alkaline seawater electrolysis. The N@C-Ni_1-Fe_5/NF exhibits η of 331 mV (85 $mVdec^{-1}$) for OER and 115 mV (73 $mVdec^{-1}$) for HER to achieve 10 mA cm^{-2} (without iR correction). TOF of N@C-Ni_1-Fe_5/NF (OER: 0.0624 s^{-1}/IrO_2/NF - 0.0185 s^{-1}; HER: 0.0382 s^{-1}/Pt/NF - 0.0843 s^{-1}) was found to be higher than IrO_2 and near to Pt, respectively. The N@C-Ni_1-Fe_5/NF displays durability of 50 h with potential loss of 3.2% (OER) and 3.0% (HER). Alkaline water electrolyser of N@C-Ni_1-Fe_5/NF//N@C-Ni_1-Fe_5/NF required only 1.66 V for effective water splitting and stable over 50 h with low potential loss of 3.5 %. In solar to hydrogen water splitting, the solar cell structure of N@C-Ni_1-Fe_5/NF requires 1.65 V for non-stop evolution of H_2 and O_2, allowing low-cost, large-scale hydrogen generation.

Keywords: Seawater electrolysis Oxides; Solar-driven electrolyzer; OER and HER.

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Thermochemical Influence of Activating Flux Powders on TIG Weld Penetration Depth in 316L Stainless Steel

Dhayaal B Chungath[1], **Mohammad Fiam K M S[1]**, Abhiram T A[1], Vishnu S Nair[1], Aju Agustine[1], K A Abdul Vahab[1], Mebin T Kuruvila[2], Anoop K Unni[2, *]

[1] *Department of Chemical Engineering, Amal Jyothi College of Engineering, Kanjirappally, Kerala, 686518, India.*

[2]*Department of Metallurgical and Materials Engineering, Amal Jyothi College of Engineering, Kanjirappally, Kerala, 686518, India*

*Corresponding Author E-mail: anoopkunni@amaljyothi.ac.in

ABSTRACT

This study investigates the chemical interactions that occur between activating flux powders and the metal on the surface of the weld pool when welding 316L stainless steel (SS) plates using Activated-TIG welding (A-TIG). It has been found that using activating flux powders during A-TIG welding of stainless steel increases penetration depth and creates stronger welds. By analyzing chemical kinetics at the weld interface, these fluxes tend to increase the rate of metal melting and fusion. The fluxes lower the system's Gibbs free energy thermodynamically, improving the efficiency of the welding process. Activating flux powders are a useful supplement to TIG welding procedures for stainless steel because of their dual effect of enhanced chemical kinetics and thermodynamics which ensures better weld quality and productivity. Five distinct oxide-based flux powder combinations mainly SiO_2, CuO, MnO_2, MoO_3 and Al_2O_3 were used in this investigation. A-TIG welding experiments were carried out one of which was flux-free. Different amounts of dissolved oxygen were added to the weld pool by varying the oxide flux components, which resulted in variations in the weld pool properties. To investigate the chemical reactions between the fluxes and weld pool, weld slag XRD analysis and Gibbs thermodynamic calculations were performed. Results show that arc constriction is significantly influenced by the kind of chemical reaction that occurs between the flux and the metal in the weld pool.

Keywords: Activated-TIG welding; Chemical kinetics; Gibbs Free energy; 304L SS; Weld pool.

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Comparative Study on Hydroxyapatite Coated Titanium Substrates

Dheeraj Dev V D*, Girinandini M, Adithi Sasi, Adithyan Ajikumar, Sajith Babu C, Rahul N U

Department of Mechanical Engineering, Government Engineering College Thrissur, Ramavarmapuram 680009, Thrissur, India.

*Corresponding Author Email: dheerajdev555@gmail.com.

ABSTRACT

The project presents a comprehensive comparative study on titanium substrates subjected to various coating methods, with a primary focus on elucidating the influence of these coatings on surface characteristics. This research involves the application of hydroxyapatite coatings through different techniques which includes paint brush method and spin coating method. Hydroxyapatite coating was synthesized as suspension of hydroxyapatite in oil of turpentine and also synthesized via water-based sol gel. The aim is to understand and compare the efficacy of these coating methods in enhancing the properties of titanium substrates for potential application in biomedical implants. Surface characteristics encompassing morphology, crystalline phases, elemental composition, wettability and cytotoxicity will be thoroughly investigated. For surface characterisation, the surfaces were investigated by scanning electron microscope and EDAX. And it shows that water-based sol gel shows uniform coating than the turpentine oil solution used. Also spin coating was more efficient in providing uniform coating and better adhesion than paint brush method. Wettability was checked using contact angle method and the result shows spin coating method provides more hydrophilicity than paint brush method. Cytotoxicity was evaluated using DLA (Daltons Lymphoma Ascites) test and cytotoxicity range of water-based sol gel indicates its suitability for application of coating on implants.

Keywords: Titanum; Hdroxyapatite; EDAX; DLA; Cytotoxicity.

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Phase Change Material-Based Cooling for Thermal Management of Drum Brakes

Keerthana Unnikrishnan E[1], Neha Catherine Anil, **Swinkle Rose**, Akbar S, Sajith V*

Department of Materials Science and Engineering, National Institute of Technology Calicut-673601, Kozhikode, Kerala, India

*Corresponding Author E-mail: sajith@nitc.ac.in

ABSTRACT

Drum brakes are commonly employed in large trucks and buses, and their effective thermal management is crucial for optimizing heat dissipation, enhancing brake performance, and prolonging the lifespan of brake shoes. The present work focuses on applying phase change material (PCM) to improve the heat dissipation from the drum brake system. The study involves the selection of a suitable PCM based on the maximum operating temperature of the drum brake and the incorporation of PCM in the drum brake for heat removal during braking. Eicosane and Docosane were selected as the PCM and were characterized by Differential Scanning Calorimetry and Thermogravimetric analysis to obtain the thermal properties. A composite PCM was prepared using Eicosane and Docosane, filled in stainless steel tubes, and fixed to the brake shoes. The experiments were conducted in the test setup using the brake drum with and without PCM incorporation and the temperature of the brake lining was measured and compared. The temperature of the brake shoes was found to be dropped by 8^{o}C with the incorporation of PCM in the brake shoes. Experimental analyses were conducted, revealing a significant reduction in the temperature of the brake shoe and liner components of the drum brake system. This study is an innovative solution to the heat failures of current drum brake systems in the automotive industry.

Keywords: PCM; Drum brake; Heat dissipation.

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Transdermal Patch using Biocompatible Carboxymethyl Hexanoyl Chitosan for Therapeutic Delivery of Vitamin D

Sathish Kumar M K, Sudhakara Prasad*

Nanomaterial Research Laboratory, Smart Materials And Devices, Yenepoya (Deemed to be University), Deralakatte, Mangalore - 575 018, India

*Corresponding Author E-mail: ksprasadnair@yenepoya.edu.in

ABSTRACT

Vitamin D deficiency is a widespread health issue affecting millions globally, leading to various health problems such as weakened bones, impaired immune function, and increased risk of chronic diseases. Traditional methods of addressing this deficiency, such as oral supplements, often face challenges related to absorption and patient compliance. Herein, a novel transdermal patch designed to deliver Vitamin D efficiently through the skin. The patch utilizes biocompatible carboxymethyl hexanoyl chitosan (CHC) to enhance permeation and ensure effective delivery of the active form of vitamin D. The invitro studies are carried out with HaCaT cell lines includes cytotoxicity testing, permeation studies, and bioavailability assessments. In addition, skin permeation studies and delivery studies are performed with artificial membranes. The results demonstrate that the as developed dermal patch have the potential to provide an effective and convenient solution for managing vitamin D deficiency, offering improved patient compliance and enhanced therapeutic outcomes.

Keywords: Vitamin D deficiency; Transdermal patch; Carboxymethyl hexanoyl chitosan; Drug delivery.

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AB 286

Photo-assisted capacitive performance of Vanadium based supercapacitor

Hridya C Prakash[1], Sudip K Batabyal*

Department of Physics, Amrita School of Physical Sciences, Coimbatore, Amrita Vishwa Vidyapeetham, Tamil Nadu, India

*Corresponding Author E-mail: *s_batabyal@cb.amrita.edu*

ABSTRACT

Developing highly efficient solar cells merged with rechargeable energy storage systems is the key to accomplishing a sustainable future in the energy sector. Also, the global demand for energy concerning the depletion of fossil fuels has raised significant breakthroughs in developing green and clean energy resources. One of the most easily accessible energy sources on Earth is solar energy. Solar energy can be converted into electrical energy using solar cells. However, this harvested energy must be stored in a storage system like a battery or supercapacitor to supply electrical energy steadily in the desired quantity at the desired time. Solar cells are usually connected to an electrochemical capacitor or rechargeable batteries, which adds cost and complexity to the system. To address this problem, a material capable of harvesting and storing energy could reduce the cost and lessen the unpredictability of energy related to solar technologies. Therefore, we propose an energy storage system that can be directly charged by sunlight without external solar cells. Semiconductors are integrated into electrochemical energy storage systems to convert solar to electrical energy, which requires no additional circuitry to convert and store energy . Ideally, combining energy harvesting and storage in a single device would remarkably improve their volumetric performance. Photoactive materials like vanadium pentoxide can be used for these applications. Herein we have synthesized 1D vanadium-based nanostructure and fabricated symmetric devices using this material. There was an increase in capacitance in the presence of light. The increase in capacitance value in the presence of light is a clear indication that the photo charging-based supercapacitor will pave an innovative path in constructing futuristic energy storage devices.

Keywords: Photoelectrode; Photo supercapacitor; Vanadium pentoxide; Coin cell; Symmetric device.

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Microstructural Characteristics, Mechanical and Wear Behaviour of Nano Hexagonal Boron Nitride Reinforcement in Aluminium Metal Matrix Composites

Nice Menachery[1,2], Shijo Thomas[1,*], B. Deepanraj[2] and Lijo P Thomas[3]

[1] *Department of Mechanical Engineering, School of Engineering and Technology, CHRIST University, Bangalore, 560 074, India*

[2] *Department of Mechanical Engineering, Jyothi Engineering College, Thrissur, India*

[3] *Department of physical sciences, Kristu Jayanti College, Bangalore, 560077, India*

*Corresponding Author E-mail: Shijo.thomas@christuniversity.in

ABSTRACT

Aluminium metal matrix composites (AlMMC's) are used in most of the industries due to their excellent properties which includes better high strength to weight ratio, better thermal and electrical conductivity. The limitations of the Aluminium alloys (AA) are generally modified by the incorporation of reinforcements both organic and inorganic types. Commonly, ceramic reinforcements such as Al2O3, SiC, MoS2 etc. are reinforced into Aluminium alloys (AA) at different weight percentages. Less number of studies were reported which reinforces hexagonal boron nitride (hBN) into the metal composites. In this study, we look upon the microstructural, mechanical and wear behaviour of AlMMC's fabricated by stir casting method, by reinforcing nano hexagonal boron nitride. AA7050, the high strength alloy which is used in the structural applications are chosen as the matrix. The property degradation of the AA 7050 can be successfully eradicated by adding hBN which is a very hard. The composite was manufactured for different weight percent's of hBN ranging from 0 to 2 wt. %. The prepared composite was subjected to various tests such as microhardness, tensile, compression, impact strength and wear test. Microstructural analysis was done using FESEM. The resultant hBN reinforced aluminum composites exhibit improved microhardness, tensile strength, compressive strength and impact strength. In comparison to unreinforced aluminium alloys, 2 wt.% of hBN reinforcement enhanced the hardness by 20 %, tensile strength by 25%, the compressive strength by 15%, the impact strength by 153% and wear rate by 12% at higher load.

Keywords: Nano composites; Aluminium; Hexagonal boron nitride (hBN); Aluminiuim alloy.

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Investigation of Doped SBNT Ferroelectric Materials for High-Efficiency Energy Storage Application

Neetdhulakshmy M N[1], Sudheendran K[2,*]

Research Department of Physics, Sree Kerala Varma College, (University of Calicut), Thrissur-680011, Kerala, India

*Corresponding Author Email: neetdhulakshmy9@gmail.com

ABSTRACT

This research investigates the properties of SBNT-based ferroelectric materials, focusing on energy storage density and dielectric characteristics. The chemical compositions studied include $Sr_{0.6}Bi_{0.2}Na_{0.2}TiO_3$ and its doped forms $Sr_{0.6}Bi_{0.2}Na_{0.2}TiO_{3-x}ZnO$ (where x = 0.02, 0.03, 0.04). Variations in these compositions were explored across different temperatures. Synthesized through the solid-state reaction method, X-ray diffraction (XRD) analysis reveals a pseudo-cubic structure, while the Scherrer equation was used to calculate crystallite size, which decreases with increased doping levels. Band gaps, ranging from 3.23 to 3.72 eV, were determined using the Tauc method from UV-visible spectroscopy. The dielectric constant and loss were examined via impedance analysis, and photoluminescence characteristics were assessed. Morphological insights were obtained through scanning electron microscopy (SEM), and structural details were elucidated via Raman spectroscopy. This study underscores the potential of SBNT to enhance energy storage efficiency and reduce costs in future applications.

Keywords: Ferroelectric materials; Solid-state reaction method; Energy storage; SBNT; Dielectric properties.

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Sonoelectrochemical Synthesis of ZnO Nanoparticles for Supercapacitor Electrodes

Sreya O V, T Sivasankar

Department of Chemical Engineering, National Institute of Technology Tiruchirappalli, Thuvakudi, Tiruchirappalli, Tamil Nadu, India

*Corresponding Author E-mail: ssankar@nitt.edu

ABSTRACT

Energy storage devices hold a prominent role in today's world. If these devices are synthesized with high energy density in addition to power density, then their importance quadruples. In order to enhance the properties of supercapacitors, innovations in the electrode and electrolyte are necessary. Electrodes made of nanoparticles have shown positive changes in the operation of supercapacitors. Especially, metal oxide nanoparticles like nickel, zinc, chromium, etc show high specific capacitance, good electrochemical stability and ability to undergo fast redox reactions due to their large surface area. In this study, zinc oxide (ZnO) nanoparticles were synthesized by electrochemical method in assistance with ultrasound. When ultrasound was combined with electrochemical method the individual disadvantages like high synthesis time, lower yield, uniform morphological characteristics, etc are overcome. For this, zinc plates are used as electrodes and sodium bicarbonate is used as electrolyte solution. In order to achieve the desired nanoparticles, the synthesis process is optimized by varying ultrasound power, ultrasound time, voltage and electrode distance. The synthesized nanoparticles were characterized by TGA, FTIR, XRD and SEM. The obtained ZnO nanoparticles was found to be thermally stable, pure from the FTIR and XRD analysis, and its size ranges from 70 to 95 nm. The ZnO nanoparticles were then used to form electrode for supercapacitor application where KOH was used as an electrolyte. Electrochemical studies of the supercapacitor were performed using cyclic voltammetry, galvanostatic charge-discharge studies and capacitance retention. When compared to supercapacitor made from electrochemical synthesis, the supercapacitor made from sonoelectrochemical method proved to provide higher performance.

Keywords: Nanoparticle; Supercapacitor; Energy.

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Effect of Particle Size of TiO_2 in Polymer Composites Used in Triboelectric Nano Energy Harvester

Baby Sreeja S D*, Abhinandh Suresh, Atul Krishna Nair, Gautham Jayesh, Krishnaraj C P, Prithvi P Madhu, Sundararaman Gopalan, Sreenidhi Prabha Rajeev, O D Jayakumar

Department of Electronics and Communication Engineering, Department of Wireless Networks and Applications, Amrita Vishwa Vidyapeetham, Amritapuri

*Corresponding Author E-mail: babysreeja@am.amrita.edu

ABSTRACT

This study explores the potential of integrating titanium dioxide (TiO_2) particles into polymer composites to enhance the performance of triboelectric nanogenerators (TENGs). The triboelectric nanogenerators can be optimised for energy harvesting efficiency. Due to its high work function, TiO_2 facilitates efficient electron transmission in energy harvesters and improves the intensity of charge production during contact. TiO_2's durability, low operating costs and energy gathering capabilities make it an essential part of energy harvesters. Utilising TiO_2 particles within a Poly-Dimethyl siloxane (PDMS) polymer matrix, the energy generating layer is prepared. To maximise the effectiveness of energy harvesting materials, different sizes of TiO_2 particles, including nano and micro particles, were employed. In a variety of energy harvesting systems, smaller particle sizes result in greater surface area, based material characteristics, and enhanced energy conversion efficiency. Considering the effect of particle size of TiO_2 in polymer composites used in TENG, the nanoparticles exhibited better triboelectric and electrical properties. Experimental testing, involving both manual and mechanical tapping, demonstrates the device's ability to generate electrical energy, yielding 5.12 volts (manual tapping) and 5.8 Volts (mechanical tapping). The proposed device fabricated with PDMS + TiO_2 nanoparticle film successfully powered a digital calculator and a digital watch. These findings highlight the potential of the hybrid polymer nanocomposite TENG device for integration into future self-powered, energy-harvesting, low powered devices.

Keywords: Tribo- Electric Nanogenerator (TENG); PDMS polymer; TiO_2 micro and nano particles; Hybrid polymer nanocomposite.

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Impact of MnO_2-Doped $BaTiO_3$ Compositional Variations in PDMS Polymer Composite Thin Films for Enhanced Triboelectric Energy Harvesting

Baby Sreeja S D, Lauksiga M P, Simla Simson, Lakshmi Nanda, Sreenidhi Prabha Rajeev, Sundararaman Gopalan

Department of Electronics and Communication Engineering, Amrita Vishwa Vidyapeetham, Amritapuri, Kerala, India

*Corresponding Author Email: babysreeja@am.amrita.edu

ABSTRACT

Triboelectric energy harvesting systems uses suitable materials to convert vibrational energy into electrical output. Utilizing an economical hydrothermal technique, flexible triboelectric films composed of $BaTiO_3$/PDMS micro-composites are fabricated for energy harvesting applications. Barium Titanate ($BaTiO_3$) ceramic powder and polydimethylsiloxane (PDMS) polymer are combined in a 4:1 weight ratio to form the ceramic-polymer composite film. Triboelectric devices generally have low current density, despite their many desirable qualities, including high energy density, small weight, and compact design. This problem is reduced by doping the $BaTiO_3$/PDMS micro-composites film with Manganese dioxide (MnO_2), which is positioned at the negative end of the triboelectric series, which enable the composite to gain electrical charge through friction, when in contact with materials in higher position in triboelectric series. So, the ceramic-polymer composite is then doped with varying weight percentages of Manganese Dioxide (MnO_2) to enhance its dielectric properties and enhanced electron transfer capabilities. The fabricated flexible $BaTiO_3$/PDMS micro-generator film and the Mn incorporated $BaTiO_3$/PDMS film were cut into square shape for $BaTiO_3$/PDMS Tribo generator device and for $BaTiO_3$/PDMS/ MnO_2 Tribo electric microgenerator device. Copper conductive adhesive tape was pasted on both sides of the film. The fabricated micro-generators consist of 3 layers, the copper films at the top and bottom acts as the electrodes, and the MnO_2 doped $BaTiO_3$/PDMS micro- composite act as the Tribo electric potential generator under external excitations. The triboelectric properties of these devices are subsequently characterized and evaluated. MnO_2 doping improves the dielectric properties and enhanced electron transfer capabilities of $BaTiO_3$, resulting a device that, when subjected to vibrational energy, generates significant output voltages while maintaining flexibility, heat resistance, and stretchability.

Keywords: Triboelectric energy harvesting; Manganese Dioxide (MnO_2); Enhanced electron transfer capabilities; MnO_2 doped $BaTiO_3$/PDMS micro-composites.

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Light Confinement in an Ordered and Disordered Superlattice Structure

Ravi Kumar Bharati , Ashiq K M , Anirban Sarkar*

Department of Physics, National Institute of Technology Calicut,

Kozhikode, Kerala - 673 601, India,

*Corresponding Author E-mail: anirban@nitc.ac.in

ABSTRACT

Superlattice is a photonic device formed by stacking two or more different photonic crystal (PC) structures in a periodic arrangement. In a superlattice, each constituent PC is called a subcell whereas the repeating unit is termed a supercell. In this work, we investigate the propagation of electromagnetic (EM) waves through a superlattice structure and its constituent one dimensional (1D) PCs which are different from each other. Transfer matrix method is employed to numerically simulate the reflection/transmission spectra of these structures. In a completely ordered scenario, the superlattice structure supports the photonic stop-bands corresponding to both of the PCs. For further investigation, different strengths of randomness are introduced in the thicknesses of the crystal-layers. We observe that despite the reflection spectra being different for different constituent PCs, they are modified by the randomness in a similar manner. However, for randomized superlattice, photonic stop-band features of its reflection spectrum are diminished much faster with the strength of the randomness compared to that of randomized PCs, generating a more flattened broad-band reflection spectrum for the superlattice structure. These results would be useful for developing different opto-electronic devices such as filters and oscillators.

Keywords: Photonic crystal; Randomness; Superlattice.

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Design and Analysis of a Rigid Flange Coupling for the Propulsion of Houseboat

Parvathy S Pillai[1], Rajesh P Nair[1,*]

Department of Ship Technology, Cochin University of Science and Technology, Kochi, Kerala, India

*Corresponding Author E-mail: rajeshpnair@cusat.ac.in

ABSTRACT

This paper presents the design and finite element analysis (FEA) of a marine rigid flange coupling for a traditional house-boat plying in Alleppey backwaters, capable of transmitting a power of 60 hp at 800 RPM. The vessel is currently under a retrofitting process for environmental friendly and sustainable backwater tourism. Various house-boat electrification projects are becoming more popular in an attempt to reduce the usage of fossil fuel. In order to improve energy efficiency and to minimize environmental impacts arising out of marine propulsion systems, this paper focuses for energy efficient performance by using industrial standard materials such as Stainless Steel 316, plain carbon steel, aluminium, and grey cast iron. The materials chosen will facilitate to reduce the timely maintenance and to extend life cycle of the components, subsequently it reduces the conventional cost for a marine flange coupling. Additionally, by ensuring that the materials are recyclable, it guarantees to reduce the carbon footprint. Couplings are mechanical components pivotal for power transmission, playing a vital role in traditional, electric, and hybrid marine engines. The geometry is modelled using CATIA5 and the finite element analysis is done using Abaqus, analyzing the stress distribution and displacement under standard operating conditions. The model is optimized by exploring with several material combinations. For example, flanges and hub are designed with grey cast iron while the keys, nuts and bolts use Stainless Steel 316. The integration of these materials offers the marine rigid flange couplings with corrosion resistance and enhanced durability. Through optimization, fuel efficiency can be enhanced, eventually leading to a reduction in the emission of greenhouse gases from conventional marine engines. The findings indicate that material optimization reduces the concentration of stress, and stainless steel 316 is the ideal material among those selected. The study further explores on how it will influence on an electric propulsion systems, which are currently standing out for their remarkable contribution in minimised environmental impact. This application incorporates energy-efficient and environmentally sustainable mechanical component design into the marine sector.

Keywords: Energy-Efficiency; Optimisation; Eco-friendly; Sustainability; Propulsion.

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Phase Transition Study of Sn Doped GeTe for Phase Change Memory Applications

Mubaris N K, Rajkumar Shanajoba Singh, Vinod E Madhavan*

Department of Materials Science and Engineering, National Institute of Technology, Calicut, Kerala, India

*Corresponding Author Email: vinodem@nitc.ac.in

ABSTRACT

Chalcogenide based phase change memories are considered for next generation Phase Change Random Access Memory (PCRAM) applications because of their unique reversible crystallization and amorphization properties. GeTe is one of the known compound for PCRAM for their higher crystallization temperature and thermal stability. A novel compound is designed to substitute Ge with Sn to reduce the cost and overall melting temperature of the system for find the suitability for memory applications. The compound $Ge_{1-x}Sn_xTe$ with x =0,0.5 were prepared by melt fusing method and thin films were deposited out of it using the thermal evaporation technique. The as-deposited films are amorphous as verified by XRD. The insitu resistance vs temperature measurements show the transition temperature of GeTe is 150 ^oC and $Ge_{0.5}Sn_{0.5}Te$ is 110 ^oC with a contrast of 6 and 5 orders of magnitude respectively. Though both alloys can be used for memory applications with their district phase contrast, the presence of Sn replacing Ge seems to reduce the stability of the GeTe compound. The reduction of transition temperature may affect the thermal stability of the compound; however a lower transition temperature may reduce the SET power requirements for PCRAM applications. This study also show that this novel compound design can be used for electrical resistance contrast tuning which can be of formidable importance for the neuromorphic computing applications.

Keywords: Phase change materials; PCRAM; Phase formation.

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Corrosion Inhibition Prospective of Collagen Zinc Oxide Nanocomposite Coating on Mild Steel in an Acidic Medium

Shamnamol G K[1,*], Manjima Mohan[1], Sam John[2]

[1]*Department of Biotechnology & Biochemical Engineering, Sree Buddha College of Engineering, Pattoor, APJ Abdul Kalam Technological University, Kerala, India*

[2]*Research and Post Graduate Department of Chemistry, St. Berchmans College, Changanassery, Kottayam-686101, Kerala, India*

*Corresponding Author E-mail: gkshamna@gmail.com

ABSTRACT

Corrosion imposes a momentous menace to the integrity and longevity of metal infrastructures, leading to substantial economic losses and safety hazards worldwide. In acidic environments, corrosion rates are particularly accelerated, exacerbating the need for effective corrosion inhibition strategies. An efficient and cost- effective way to prevent corrosion damage is by using efficacious organic coatings. Nanoparticles (NPs) exhibit diverse size and shapes that have been implemented to elevate the engineering proficiency of coatings. This study addresses the critical importance of corrosion inhibition by investigating the efficacy of a collagen-zinc oxide (Col/ZnO) nanocomposite coating applied to mild steel substrates exposed to a corrosive 1 M HCl solution. Synthesized zinc oxide nanoparticles, sourced from banana peduncle extracts, were integrated into the nanocomposite alongside collagen for enhanced structural integrity and corrosion resistance. The coating was prepared and applied to mild steel using a sol-gel method and Dip coating strategy respectively. The nanocomposite is then emblemized by Fourier Transform Infrared Spectroscopy (FTIR) and Thermogravimetric analysis (TGA). In the present investigation, ZnO NPs biosynthesized using banana peduncles were analysed by FTIR, UV-visible spectroscopy, X-ray diffractometer analysis (XRD), and Transmission Electron Microscopy (TEM). Electrochemical Impedance Spectroscopic studies (EIS) and Potentiodynamic Polarization (PDP) techniques were employed to scrutinize the anticorrosive behaviour of the coated mild steel specimens.

Keywords: Collagen Zinc Oxide nanocomposite; Corrosion inhibition; Mild steel; Organic coating.

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Affordable Colorimetric Paper Sensor for the Early Detection of Cancer Biomarker

Ziba Rasheed, K Sudhakara Prasad*

Nanomaterial Research Laboratory, Smart Materials And Devices, Yenepoya (Deemed to be University), Deralakatte, Mangalore 575 018, India

*Corresponding Author E-mail: ksprasadnair@yenepoya.edu.in

ABSTRACT

The development of novel cancer treatments has increased survival chances for the patient, and on the other hand dramatically increasing the cost per patient. It is necessary to have prompt detection techniques for cancer positive patients to reduce the economic burden and increase access to early treatment .The need for REASSURED (real-time connectivity, ease of specimen collection, affordable, sensitive, specific, user-friendly, rapid, and robust, equipment-free, and deliverable to end-users) criteria by WHO point towards paper based analytical devices as point-of-care test (POCT) platform. Urokinase-type plasminogen activator (uPA) is one of the biomarkers for early detection of cancer. The up regulation of uPA, leading to the proteolytic degradation of the extracellular matrix (ECM), is a key biological process that drives tumor cell motility and progression towards the characteristic invasive phenotype observed in metastatic cancers like breast, ovarian, colorectal and lung cancers. Serum-based paper analytical device for colorimetric detection of the said cancer biomarker follows the principle of immuno-sandwich assay on a paper platform, exploiting the specificity of antigen – antibody interaction to achieve high sensitivity and specificity. In order to develop the sensor we have utilized the monoclonal antibodies and nano-bioconjugates for signal enhancement. The output in the form of color intensity not only facilitates naked eye detection but also gives opportunity for the quantifiable estimation of biomarker present in the serum .The rapid results received within minutes help in early prognosis, reducing the turn-around-time for cancer detection.

Keywords: Urokinase-type plasminogen activator cancer; Immuno-sandwich assay; Colorimetric detection; Signal enhancement.

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Understanding the Phase Transition of $FAPbI_3$ Thin Films for Enhanced Solar Cell Performance

Sanjeev Sajan, Shana Sudhakaran, Nidha C, Vinod E Madhavan*

Department of Materials Science and Engineering , National Institute of Technology Calicut,NIT Campus P.O 673601,Kozhikode, India.

*Corresponding Author Email: vinodem@nitc.ac.in

ABSTRACT

Perovskite solar cells have garnered significant attention due to their potential for achieving high efficiencies at a low cost.Formamidinium lead iodide ($FAPbI_3$) is a promising material for this application owing to its narrow bandgap and high thermal stability. However, the phase transitions at ambient atmosphere, particularly from the photoactive black α-phase to the non-photoactive yellow δ-phase, remains a critical challenge. This study investigates the structural and optical properties of $FAPbI_3$ thin films annealed at different temperatures (125, 150, and 175 °C) to determine the factors influencing phase transition. Temperature dependant Raman (LINKAM) study is conducted on FAPI from –150 ^{o}C to 250 ^{o}C to further understand the insitu phase transition from cubic photoactive black α-phase to non-photoactive yellow δ-hexagonal phase. Three Raman active modes cantered at 63 cm-1,96 cm-1,114 cm-1 indicating the presence of δ-phase upto 150^{o}C, while at 150^{o}C a transition from δ-phase to cubic α-phase. The Tauc plot obtained from the UV spectrum revealed a bandgap of 1.49 eV which is ideal for solar cell applications. XRD showed the presence both cubic and hexagonal mixed phases in samples annealed up to 150^{o}C, with more cubic phases above 150oC. An additional peaks from lead iodide was visible, indicating the decomposition of the sample at higher temperatures. A better understanding on the structural rearrangements can help to design strategies to control phase transitions and improve the long-term performance of $FaPbI_3$ based perovskite solar cells.

Keywords: $FAPbI_3$; XRD; RAMAN; Perovskite.

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Structural and Optical Characterization of Entropy-Stabilized Rare Earth-Hafnate Pyrochlore Oxides

Gaius Cherian Mathew and Shijo Thomas*

Department of Materials Science and Engineering, National Institute of Technology,

Calicut, Kerala, India

*Corresponding Author E-mail: shijo@nitc.ac.in

ABSTRACT

Entropy-stabilized oxides find application in several areas due to their interesting properties which comes from their 4 core attributes. Here we have developed 5 different entropy-stabilized pyrochlore oxides, with 4 rare-earth (RE) elements and a transition metal (TM), $4RE_2TM_2O_7$. Their structural as well as optical properties is studied in this work. A 4-element combination from La, Ce, Pr, Nd and Gd are selected as REs and Hf is taken as the TM. The 5 novel phase-pure oxides are synthesized using a solution combustion method using urea as fuel. The combustion products are calcined at different temperatures up to 1600°C, to study the phase stability. Structural characterizations like X-Ray Diffraction (XRD) and Raman confirms the formation of single phase pyrochlore oxides. All 5 developed oxides exhibit excellent phase stability up to 1600°C. The morphology and elemental compositions are studied utilizing Scanning Electron Microscopy (SEM) equipped with Energy Dispersive Spectroscopy (EDS). The theoretical density and lattice parameters are optimized using Rietveld refinement of the developed oxides. To study the optical properties, UV-Visible Diffuse Reflectance Spectroscopy (DRS) is studied across a wavelength range of 200-800nm. The Kubelka-Munk plots of developed oxides reveal narrow bandgaps ranging from 1.75 to 2.67eV. Thus in this work, we have developed 5 novel phase-pure, entropy-stabilized RE-TM pyrochlore oxides with great phase stability and narrow bandgaps.

Keywords: Entropy-Stabilized Oxide; Medium Entropy Oxide; Pyrochlore; Narrow bandgap; Rare Earth Hafnate.

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Coconut Shell Biocomposite for Cutlery Application

Joel Antonie Harock, Faheem M V, Parwon Manoj, Soney Varghese, C N Shaym Kumar*

Department of Materials Science and Engineering, National Institute of Technology Calicut, Kozhikode, Kerala 673601, India

*Corresponding Author E-mail: shyam@nitc.ac.in

ABSTRACT

Polymers are widely used because of their versatility, durability, and ability to shape them into different forms. Most of the commercially used polymers are non-biodegradable and environmentally harmful. We can use biocomposite, especially from agricultural byproducts like coconut shells as an alternative to single-use plastic. In such a context, this work discusses using coconut shell powder (CSP) to fabricate a biocomposite as a replacement for single-use plastic in cutlery. The method involves acetic acid pretreatment followed by hot pressing at high pressure. This method removes the need for an external binder for the fabrication of the biocomposite. Optimum properties were achieved by using the treatment with 20 wt.% acetic acid and an average particle size of 212 µm. This combination resulted in a biocomposite with mechanical stability and reduced porosity. The proposed fabrication method allows the reshaping of biocomposite, thereby enhancing its recyclability. Our study suggests that the fabrication of biocomposite form CSP can be used as a substitute for petroleum-based polymers for reusable cutlery applications. This also converts agricultural waste into value-added materials. It offers a practical solution to environmental pollution and advances innovation in sustainable consumer goods.

Keywords: Coconut shell powder; Biocomposites; Sustainable materials; Eco-friendly cutlery; Internal binder.

AB 308

Investigation of Rayleigh, Love, Sezawa SAW modes for the Selective Determination of Chlorinated Hydrocarbons

Anoop A V[1], Bhargav Panchal, Soney Varghese

Nanomaterials & Devices Research Laboratory, Department of Materials Science and Engineering, National Institute of Technology Calicut- 673601, Kerala, India

*Corresponding Author E-mail: anoopsmse@gmail.com

ABSTRACT

Chlorinated hydrocarbons used in a variety of industrial and domestic purposes have been attributed to multiple harmful health problems including cancers following long term exposure. VOC gas sensors utilize advanced technology to detect these gases, and hence can monitor air quality, and help to mitigate risks. Among various sensors used for detection and quantification of these gases, SAW sensors present multiple advantages. In this study Rayleigh, Love, Sezawa modes of SAW waves for the selective determination of chlorinated hydrocarbons are investigated and compared using COMSOL Multiphysics software. The piezoelectric layer taken is lithium niobite with different orientations, atop which a pair of interdigital transducers (IDTs) made from aluminium, was patterned. The electrodes are approximately assumed as infinitely thin and massless to simplify the computation. Polyisobutylene (PIB) that has high selectivity and greater reversibility in terms of adsorption and desorption, was selected for the gas-sensing layer. Silicon dioxide (SiO_2)- that offers low damping, sufficient low shear velocity and excellent chemical and mechanical resistance and is used as a guiding layer. A customised mesh with respect to the wavelength is used. Unit cell optimization for different waves was done using changes in thickness of guiding layer, electromechanical coupling coefficients, resonance and anti-resonance frequencies of substrate. From the linear frequency shift the selectivity is determined and compared for the three modes of SAW devices.

Keywords: Surface Acoustic Waves; Chlorinated hydrocarbons; COMSOL multiphysics; Sensitivity.

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TGA Studies of *Hevea Brasiliensis* Leaf Biomass for Energy Extraction

A Fazil[1,*], Vaishakh Nair[2], Jeevandersh S[1], Athira Chandran G[1],

Hari Govind A[1], Gopika O S[1]

[1]*Department of Chemical Engineering, TKM College of Engineering, Kollam, 691005, Kerala, India*

[2]*Department of Chemical Engineering, National Institute of Technology Karnataka, Surathkal, 575025, Karnataka, India*

*Corresponding Author E-mail: fazil@tkmce.ac.in

ABSTRACT

Hevea brasiliensis (Rubber Tree), a deciduous tree with annual leaf fall, is the primary source of natural rubber. The dead leaf of the tree is a waste material that can be considered as a biomass for the production of energy through thermochemical methods including pyrolysis and gasification, which requires the kinetic data of pyrolysis reaction. The present study focuses on the thermal behaviour of *Hevea brasiliensis* leaves using thermogravimetric analysis in an inert atmosphere to understand the kinetic parameters of the pyrolysis reactions, considering the heating rates from 5^0C min^{-1} to 30^0C min^{-1} and temperature from 30°C to 900°C. Physicochemical characterisations including proximate analysis, ultimate analysis, bomb calorimetry and FT-IR spectroscopy were conducted to understand the potential of the biomass for energy extraction. The physicochemical characterization revealed favourable properties of the biomass for energy production, including low moisture content, ash content, and sulphur content; as well as high volatile matter and carbon content. FT-IR analysis confirmed the presence of characteristic functional groups, while calorific value determination highlighted the high energy content of the biomass. TGA analysis demonstrated the thermal decomposition behaviour of the biomass, with distinct stages corresponding to the degradation of different biomass components. Heating rate can influence the conversion and product distribution during the pyrolysis of biomass. To understand the effect of heating rate on the decomposition of biomass, TGA runs were conducted at four different heating rates. The increase in the heating rate has not influenced the integrity of the pattern followed during the mass loss, which indicates that the overall mechanism remains unaffected with the change in heating rates. The DTG data shows that with increase in the heating rate, the decomposition rate increases. This behaviour can be established with the increase in the height and width of the DTG curves. Increase in peak height with heating rate is also an indication of complex constituents of the residue. The thermal degradation profile of the biomass shifts towards higher temperature zones with increasing heating rates. The model-independent iso-conversional methods enable the estimation of activation energy based on conversion without making any prior assumptions about the reaction model. The kinetic parameters were evaluated using four iso-conversional methods namely Kissinger-Akahira-Sunose (KAS), Ozawa-Flynn-Wall (OWF), Starink and Friedman. A range of conversion values from 0.2 to 0.6 at a step interval of 0.05 is found to give the best fit with R^2 value greater than 0.9. Heating rates of 10 °C min^{-1}, 20 °C min^{-1} and 30 °C min^{-1} were used to obtain the linear fit plots of KAS, OFW, Friedman and Starink. Activation energy of the biomass was 201.64 kJ mol^{-1}, 201.30 kJ mol^{-1}, 194.49 kJ mol^{-1}, and 223.32 kJ mol^{-1} for KAS, OFW, Starink, and Friedman method respectively. The results show that the waste dead leaf of *Hevea brasiliensis* is a potential material to be considered for energy extraction through thermochemical conversion including pyrolysis and gasification.

Keywords: Biomass; Kinetic study; Pyrolysis; Thermogravimetric analysis; Hevea *brasiliensis*; Iso-conversional methods.

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Thermal Analysis of Autogenous TIG Welding on 316LN Stainless Steel: Comparison of Contact and Non-Contact Temperature Measurements with Simulation Results

Anoop A Pillai[1], H C Dey[2], Jayadeep U B[1], Vineesh K P[1], D. Sharath[3], M Menaka[3], B Venkatraman[3]

[1]*Department of Mechanical Engineering, National Institute of Technology Calicut, Kozhikode, India*

[2]*Metallurgy and Materials Group, Indira Gandhi Centre for Atomic Research, Kalpakkam, India*

[3]*Safety, Quality & Resource Management Group, Indira Gandhi Centre for Atomic Research, Kalpakkam, India*

* Corresponding Author E-mail: anooppillai1989@gmail.com

ABSTRACT

This study presents a comprehensive thermal analysis of autogenous tungsten inert gas welding on a 316LN stainless steel plate, integrating experimental techniques and finite element simulation. Goldak double ellipsoidal heat source model is employed to simulate the heat input accurately. Experimental measurements are conducted using both contact (using K-type thermocouples) and non-contact Infrared thermography methods, comparing their effectiveness in capturing precise thermal gradients and validating the numerical predictions. The simulation achieves high accuracy, with peak melt pool temperatures and base plate temperature evolution matching the experimental results within 10%. Infrared thermography is also utilized to estimate bead width, providing valuable insights into the fusion zone width during the welding process. Additionally, the study explores the effect of varying convection heat transfer coefficient on cooling rate. This thermal analysis gives an accurate prediction of welding temperatures, providing the essential information required for subsequent residual stress analysis and for optimizing the welding parameters.

Keywords: Welding thermal analysis; Finite element analysis; IR thermography; K-type thermocouple.

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Finite Element Modelling and Experimental Validation of Temperature Evolution During the Deposition of Curved Geometry using Wire Arc Additive Manufacturing

Banala Dharmista [1], Ashok Kumar P[2], Bijoy Rajak[2], Vineesh Vishnu[1], Anoop A Pillai[1], Amit Kumar Rai[1], **K P Vineesh[1,*]**

[1]*Department of Mechanical Engineering, National Institute of Technology Calicut, Kozhikode, 673 601, India*

[2]*Tata Steel Limited, Jamshedpur, 831 001, India*

*Corresponding Author E-mail: vineesh@nitc.ac.in

ABSTRACT

Wire arc additive manufacturing process is a promising process to produce large and complex parts. In this paper, temperature evolution during the deposition of a curved geometry was studied using finite element analysis. Experiment was conducted by depositing a five layer curved geometry on a mil steel substrate plate with ER70S-6 material. Wire feed rate of 9 m/min, torch speed of 500 mm/min, and material deposition rate of 61.5 mm3/min is used for the experiment. While the deposition of geometry, temperature was monitored by using K-type thermocouple, one fixed at the centre of the curved geometry and the other away from the centre at the start of the deposition. Unidirectional deposition is used with 200s cooling between each layer deposition. Finite element model of the deposition is developed by using additive module of Ansys. Sequentially coupled temperature-displacement analysis is carried out with element activation at the melting temperature of the material. Temperature dependent material properties and convection heat loss to the environment is considered in the analysis. The results indicate the temperature evolution predicted by finite element analysis is matching closely with the experimental data with a variation of less than 15% when measured 60 mm from the centre of the curved geometry.

Keywords: Finite element analysis; Additive manufacturing; WAAM; Heat transfer.

AB 314

Development and Characterization of Gum Ghatti based Nanocomposite Reinforced with Nanocellulose Isolated from *Lantana Camara* L.

Arathi Chandran[1], Anju S Vijayan[1,*] , Athira S Vijayan[2], Vishnu R[3], Kanica Upadhyay[1], Prahlad V C[1], Ashok Kumar[1], I B Maurya[1]

[1]*Department of Forest Products and Utilization, College of Horticulture and Forestry, Jhalawar, Agriculture University, Kota, Rajasthan – 326023, India*

[3]*Department of Materials Science and Engineering, National Institute of Technology Calicut, Kozhikode, Kerala - 673601, India*

[4]*Department of Forest Products and Utilization, College of Forestry, Kerala Agriculture University, Vellanikkara, Thrissur, Kerala – 680656*

*Corresponding Author E-mail: anjucof03@gmail.com

ABSTRACT

Cellulose nanofiber has proven to be highly effective in reinforcing nanocomposite systems, especially those based on biopolymers. The properties of bio-nanocomposites developed from gum ghatti, a tree-based gum reinforced with nanocellulose derived from an obnoxious weed *Lantana camara* L. were studied. The nanocellulose isolated through acid hydrolysis method were successfully reinforced in the gum ghatti matrix at different concentrations. Bio-films were fabricated using the solution casting method and evaluated for their physical, thermal, and mechanical properties. The SEM analysis elucidated the surface morphological characteristics of the nanocomposite film. The FTIR results revealed the hydrogen bonding interactions that occurred between the gum ghatti matrix and the nanocellulose fillers, as well as the modification in chemical bonding that occurred following the interaction. The XRD analysis explained that amorphous nature of gum changed to semi-crystalline nature with the incorporation of crystalline natured nanocellulose. The effect of nanocellulose reduced the moisture content, water solubility and increased contact angle from to 44.18^o to 64.29^o, thus indicating that nanocomposite films have lower affinity than plain gum film. By adding nanocellulose to plain gum, the specific heat capacity has been reduced from 2.68 $Jg^{-1o}C^{-1}$ to 2.04 $Jg^{-1o}C^{-1}$ and raising the temperature of thermal degradation (from 208.81^{o}C to 231.37^{o}C), glass transition temperature (114.99^{o}C to 134.06^{o}C) and melting temperatures (148^{o}C to 220^{o}C), nanocellulose increased the thermal stability and thermal resistance of nanocomposites. Compared to plain gum films, the composite films demonstrated enhanced mechanical properties by improving tensile strength (1.53 MPa), young's modulus (80.47 MPa) and elastic limit (0.4 MPa) and reducing tensile strain (0.427) and elongation at break (10.16%). In general, encouraging sustainability and environmental friendliness, the incorporation of nanocellulose in the gum ghatti composites results in improved mechanical, thermal, and physical properties, thus making them promising candidate for bio-stimulant to enhance seed germination and food packaging industries and bioplastic applications.

Keywords: Nanocellulose; Gum ghatti; Bio nanocomposite film; Characterization.

AB 315

Fabrication of All Carbon Microheaters by Laser Graphitization of Photoresists

Varikkassery Jagadheesh Chandran Adarsh , Parwon Manoj, C N Shyam Kumar*
Department of Materials Science and Engineering, National Institute of Technology Calicut, Kerala, India, 673601
*Corresponding Author E-mail: shyam@nitc.ac.in

ABSTRACT

Microheaters are essential components in modern microelectromechanical systems (MEMS), finding applications in gas sensors, biomedical diagnostics, thermal management systems, fuel cells, and microreactors. They also play a crucial role in micropropulsion systems, lab-on-a-chip platforms, and advanced analytical devices such as SEM and TEM. Despite their importance, traditional metal-based microheaters face challenges related to cost, fabrication complexity, and limited reusability. This study presents a new method for fabricating all-carbon microheaters using laser graphitization of S1803 photoresists. The process involves precise optimization of laser parameters to achieve uniform graphitization, followed by selectively dissolving ungraphitized regions to create well-defined heating coil patterns. Pyrolysis was employed to enhance conductivity and thermal stability further. Raman spectroscopy confirmed high graphitic content, validating the effectiveness of the method. The fabricated microheaters demonstrated good thermal performance, achieving temperatures up to 400°C under inert conditions. This scalable and easy technique avoids the need for expensive materials and complex processes, offering a cost-effective alternative for MEMS integration and other advanced applications.

Keywords: Microheaters; Laser Graphitization; All-Carbon Microheaters; Photoresist S1803.

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Metal Oxide Based Thin Film Transistor for Hydrogen Gas Detection

Adwaidu Viswanathan, Nakka Bala Vaishnavi, Soney Varghese*

MSED, National Institute of Technology Calicut, Kozhikode, Kerala, India

*Corresponding Author E-mail: soneyva@nitc.ac.in

ABSTRACT

The detection of Hydrogen (H_2) gas using a Hydrogen sensor is described, based on the structure of a thin-film transistor. In the development of the sensor, SiO_2 layered p-type silicon substrate has been used, having doped SnO_2 as the active layer. The sensor works on identifying H_2 gas by changes in channel current as a function of time. Adsorption of hydrogen molecules on the SnO_2 active layer causes conductivity modulation through variation in carrier concentration, hence providing variation in the TFT output current. SnO_2 was deposited with varying copper doping durations of 20, 30, and 40 seconds for optimization. Scanning Electron Microscopy (SEM) analysis revealed that increasing the doping time led to a significant increase in grain size, with measurements of 20 nm at 20 seconds and 100 nm at 40 seconds. Wettability tests demonstrated a decrease in hydrophilicity with longer doping durations, where the contact angle reached 70° at 40 seconds. Gas sensing tests showed an enhanced response of 0.88% for the doped sensor, compared to 0.52% for the undoped counterpart. These findings indicate that copper doping improves the sensing performance of SnO_2-based hydrogen sensors.

Keywords: Thin film transistor; H_2 gas sensor; SnO_2 active layer; Gas sensing; Comsol-Multiphysics.

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Development of Electrochemical Sensor for the Detection of Dopamine

Shivalaya Ravi M P, Lisa Maria Malhiers, Haritha K*

Department of Materials Science and Engineering, National Institute of Technology Calicut, Kozhikode, Kerala 673601, India

*Corresponding Author E-mail: haritha_p200115mt@nitc.ac.in

ABSTRACT

This study mainly focuses on developing an electrochemical sensor platform for dopamine by using functionalized carbon nanotubes (f-CNTs) and carbon dots (C-dots). Dopamine is an important neurotransmitter whose detection is difficult due to its low concentrations and similar oxidation potentials as those of uric acid (UA) and ascorbic acid (AA). Electrochemical sensors performance highly depends on the material used for their modification. It has many advantages over traditional methods (high-performance liquid chromatography (HPLC) and mass spectrometry) like less time consuming, inexpensive, and suitable for practical applications. Carbon nanotubes have high conductivity and large surface area which contributes to an increase in electron transfer rate and adsorption of dopamine. Functionalizing dopamine leads to an increase in solubility and biocompatibility. Since C-dots have high surface to volume ratio and tuneable fluorescence they enhance the sensors selectivity and sensitivity. When combining these two materials we get a highly efficient and effective dopamine interaction. The synthesized materials are characterized using techniques like Scanning electron microscopy (SEM), Raman spectroscopy, and Fourier-transform infrared spectroscopy (FT-IR) for conformity. For the detection procedure f-CNT/C-dot was modified by drop casting it on glassy carbon electrode (GCE), where GCE is the working electrode. This whole detection process was carried on by Differential pulse voltammetry (DPV) in a buffer solution containing UA and AA. Electrochemical characterization was done for the better understanding of electron transfer kinetics and interfacial properties which was done by Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). Detection of dopamine is clearly observed which concludes that f-CNT/Cdot has high sensitivity with limit of detection (0.3 µM). Selectivity was showcased by studying the behavior of dopamine with other interfering molecules and the result is there is a negligible relative error of (<3%) in peak current which is good. The sensor showed a 30-day stability with negligible potential difference of +0.02 V and a good reproducibility with standard of deviation,0.19 µA performance indicating its good long term performance. Its practical applicability was tested by doing real life sample analysis where insulin was taken as the sample. Recovery rates ranging from 100% to 120% were obtained making it relevant study for practical scenarios like clinics or other research purposes. This project thus signifies the characteristics of f-CNT/Cdot as a good and effective electrochemical sensor platform for the detection of dopamine. The various applications related to this research are clinical diagnostics, neuroscience research, drug development and related areas.

Keywords : Dopamine detection; Electrochemical sensor; Functionalized carbon nanotubes (f-CNTs); Carbon dots (C-dots).

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Copper Nanocluster Mediated Bimodal Cancer Theranostics

Merin Joseph[1], Hanas Tharayil[1], Lakshmi V Nair[2,*]

[1]*Department of Materials Science and Engineering National Institute of Technology Calicut, Kozhikode, 673601, Kerala, India*

[2]*Mechanical and Materials Engineering Department, University of Alabama at Birmingham, Birmingham, AL 35294 (205) 975-5762 Alabama, USA*

*Corresponding Author E-mail: lvijayan@uab.edu

ABSTRACT

Metal nanoclusters have emerged as promising candidates for cancer diagnosis and therapy due to their ultra-small size and distinctive optical and photophysical properties. Their intrinsic fluorescence and ease of conjugation with therapeutic molecules make them particularly suitable for applications in bioimaging and therapy. However, single-modality treatments often fall short of achieving comprehensive cancer eradication. To address this limitation, a multi-therapeutic approach integrated with diagnostic capabilities—termed theranostics—has gained significant attention. Among metal nanoclusters, copper (Cu) remains underexplored compared to gold (Au) and silver (Ag) due to its high susceptibility to oxidation. However, its abundance, low cost, biocompatibility, and role as an essential trace element in biological systems make it a promising alternative. Herin developed a glutathione-stabilized copper nanocluster (CuC) with intrinsic singlet oxygen generation and fluorescence emission at 674 nm. To enhance its functionality, CuC is conjugated with folic acid and doxorubicin for targeted combined photodynamic therapy (PDT) and chemotherapy. The conjugated CuC demonstrated effective cancer cell imaging and therapeutic efficacy *in vitro*. Specifically, 10.5 μg (18.1 nmol) of the drug-conjugated CuC achieved 56% cell death in HeLa cells after 30 seconds of laser irradiation. This study highlights the potential of copper nanoclusters as a low-cost, biocompatible platform for targeted cancer theranostics, paving the way for effective multimodal treatment strategies.

Keywords: Copper nanoclusters; Theranostics; Bimodal therapy; Photodynamic therapy; Chemotherapy.

AB 320

Structural and Morphological Investigation of Hydrothermally Synthesized High Entropy Spinel Oxides

Abhishek Bhaisare*, Amit Bhargav, Sanjay Shrivastava and Mangesh Lodhe
Department of Materials and Metallurgical Engineering, Maulana Azad National Institute of Technology, Bhopal 462003, India
*Corresponding Author E-mail: abhishekbhaisaremonu@gmail.com

ABSTRACT

High entropy spinel oxide (HESO) is a class of materials that exhibit high configurational entropy, leading to unique structural characteristics and functional properties. Potential applications of HESOs are in energy storage devices such as Li-ion battery anode and for electrodes in Oxygen evolution reaction (OER). One of the important factors which influence the property of oxides is synthesis route, as synthesis route controls morphology of materials and which in turn affects the properties. In this study, we report the synthesis of equi-molar HESOs using different combinations of transition metals (Fe, Mn, Ni, Cu, Co, Cr, and Zn). All the synthesized materials consisted of five metals. HESOs were synthesized using hydrothermal method in the temperature range of 140-180 °C. The effect of processing parameters such as pH, temperature and type of precursors on the morphology of HESOs were studied. Nanoparticles of 40-50 nm were observed in the pH range of 9 to10.

Keywords: High entropy spinel oxide; Hydrothermal method; Li-ion battery; Morphology control.

AB 321

Phase Evolution and Characteristics of Mechanically Alloyed and Spark Plasma Sintered High Entropy Alcocrfeti Alloy

Arun Raphel[1,*], Vinoadh Kumar Krishnan[2], P Vivekanandhan[3], S Kumaran[4]

[1] *Department of Mechanical Engineering, SRM Institute of Science and Technology, Vadapalani Campus, No. 1 Jawaharlal Nehru Road, Vadapalani- 600026, Tamil Nadu, India*

[2] *Research and Development, Powder Metallurgy Division, Sundram Fasteners Limited, Hosur-635109, Tamil Nadu, India*

[3] *Centre for Automotive Energy Materials, International Advanced Research Centre for Powder Metallurgy and New Materials, Chennai, Tamil Nadu 600 113, India*

[4] *Green Energy Materials and Manufacturing Research Group, Department of Metallurgical and Materials Engineering, National Institute of Technology, Tiruchirappalli, Tamil Nadu 620 015, India*

*Corresponding Author E-mail: arunr2@srmist.edu.in

ABSTRACT

Formation of simple solid solution apart from complex inter-metallic phase made High Entropy Alloys (HEAs) unique among other alloy systems. The current study illustrates phase evolution and mechanical properties of high entropy AlCoCrFeTi HEA alloy developed using mechanical alloying (MA) and spark plasma sintering (SPS) at 45 MPa pressure and 1000℃ temperature. Mechanical alloying resulted in the evolution of a mono-phase nanocrystalline AlCoCrFeTi HEA BCC solid solution within a shorter milling time of 15 hr. During the thermal analysis, the alloy powder showed higher thermal stability without indicating melting over the entire measurement range. However, a minor FCC phase was observed during sintering. The alloy retains its nanocrystalline nature, even after sintering due to restricted grain growth and shorter sintering times. AlCoCrFeTi HEA alloy exhibits superior hardness (1091.5HV) and high compressive strength (880.02MPa) due to its inherent BCC nature and induced lattice distortion during mechanical alloying and solid solution strengthening.

Keywords: Spark plasma sintering; Mechanical alloying; High entropy alloys; Transmission electron microscopy; Scanning electron microscopy.

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Material and Design Optimization of Nature-Inspired Cellular Structures for Bioimplants

Arun Raphel[1,*], K Shunmugesh[2], Praveen A S[3], S Arun[4]

[1] *Department of Mechanical Engineering, SRM Institute of Science and Technology, Vadapalani Campus, No. 1 Jawaharlal Nehru Road, Vadapalani- 600026, Tamil Nadu, India*

[2] *Department of Mechanical Engineering, Viswajyothi College of Engineering and Technology, Ernakulam, Kerala 686670, India*

[3] *Department of Mechanical Engineering, Vel Tech Rangarajan Dr. Sagunthala R&D Institute of Science and Technology (Deemed to be University), Chennai-600062, Tamil Nadu, India.*

[4] *Department of Mechanical Engineering, NIT Campus P.O, Calicut Mukkam Road, Kattangal, Kozhikode, Kerala 673601, India*

*Corresponding Author E-mail: arunr2@srmist.edu.in

ABSTRACT

The use of porous cellular structures in bone tissue engineering can provide mechanical and biological environments closer to the host bone. However, poor internal architectural designs may lead to catastrophic failure. With the developments in the area of bone tissue engineering, the demand for new types of biomaterials is increasing. The major requirement of these materials is to possess the properties close to that of a human bone. Porous biomaterials are proved to be successful in fulfilling these requirements. Also, porous structures allow biological anchorage for the surrounding bone tissue to adhere and grow through its porous network. Topologically ordered porous structures (TOPSs) have shown great potential in biomedical application. Several designs were designed which were inspired from nature and those design were modified accordingly in order to serve the purpose. This study investigates mimicking cellular architectures to address some of the shortcomings of conventional bone implant designs. Three geometries inspired from coral, snow crystal, and microplant were designed in Autodesk Fusion 360. The compression strength and deformation response of the structures were analyzed in ANSYS using the polylactic acid (PLA) material properties. The result reveals that the coral design exhibited exceptional performance, with a maximum stress tolerance of 2760.9 MPa and a deformation threshold of 8.3 mm. The snow crystal design exhibits a stress tolerance of 174.5 MPa with a deformation limit of 4.36 mm, while the microplant design demonstrates a stress tolerance of 144.91 MPa with a deformation limit of 3.91 mm. The current research emphasis the potential of coral designs to effectively transmit stresses without premature failure for better biocompatibility.
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Keywords: Cellular structures; Topologically ordered porous structures; Finite element analysis; Compression strength.

AB 323

Development of Shape Stabilised Paraffin Wax - Graphite Composite as Thermal Energy Storage Layer in Multifunctional Floating Absorber Solar Still

Abhijith P U and Shijo Thomas*

Micro/Nanoscale Engineering Laboratory, Department of Materials Science and Engineering,

National Institute of Technology Calicut, Kozhikode - 673601

*Corresponding Author Email: shijo@nitc.ac.in

ABSTRACT

Solar desalination is a desalination technique based on thermal evaporation method. One of the major disadvantages of conventional solar still is low productivity due to bulk heating of water. Multifunctional floating absorber based solar still utilises solar interfacial evaporation technique. Here the photothermal conversion process is localized at the air-water interface so that the evaporation rate can be enhanced. Multifunctional floating absorber based solar still consists of three layers, viz: photo-thermal absorber material, water transporting layer to facilitate the water transport from the bulk fluid to the material and insulation layer to prevent the heat transfer to the bulk fluid. One factor which affects the productivity of multifunctional floating absorber solar still is the intermittent nature of the solar flux due to cloud cover, prevalent in tropical regions like India. In the present work this issue is addressed by incorporating a thermal energy storage layer to multifunctional floating absorber solar still. The thermal energy storage layer developed is a shape stabilised Phase Change Material (PCM)-Filler composite which involves paraffin wax as phase change material and graphite as thermal conductivity enhancing material. Thermal conductivity of the paraffin wax is enhanced by adding 30% Graphite powder (size less than 20 micron) to the pure paraffin wax. Paraffin wax-graphite composite exhibited a 210% increase in thermal conductivity compared to pure paraffin wax with the addition of 30% graphite powder. The encapsulation of the Paraffin-graphite composite was performed by using liquid silicone rubber. The thermal conductivity of liquid silicone rubber was further enhanced by adding 5% graphite powder.

Keywords: Multifunctional floating absorber solar still; Paraffin wax-graphite composite; Liquid silicone rubber encapsulation; Graphite powder.

AB 324

Microstructural and Failure Investigations in Thermally Aged 316 LN Stainless Steel Weld Joint under Creep−fatigue Interaction Loading

T Suresh Kumar[1*], A Nagesha [2,3]

[1] *Department of Materials Science and Engineering, National Institute of Technology Calicut, Kozhikode, Kerala – 673601*

[2] *Mechanical Metallurgy Division, Indira Gandhi Centre for Atomic Research, Kalpakkam, Tamil Nadu, India – 603102*

[3] *Homi Bhabha National Institute, Mumbai, Maharashtra, India – 400094*

[*]Corresponding Author E-mail: tsk030@gmail.com

ABSTRACT

Type 316 LN austenitic stainless steel weld joint (WJ) is thermally aged (923 K/5000 h) and investigated under strain-controlled isothermal low cycle fatigue (LCF) and peak tensile strain hold (60 s and 300 s) creep-fatigue interaction (CFI) at different temperatures between 823 K - 923 K. Cyclic softening occupied major part of the cyclic stress response (CSR) in all the tests. The CSR and fatigue life of the joint decreased with an increase in temperature and duration of hold. The failures were originated mostly in weld metal region of the joint, though the mechanism of failure was found to depend on the testing conditions. Initiation and propagation of microcracks were observed to be a combined effect of microstructural embrittlement, fatigue and creep damages, as identified through extensive microscopic examinations. Increase in the intergranular damage in here-affected zone of the joint is attributed to triple point cracks (TPCs) and their coalescence, which accelerated the crack propagation. The detrimental role of the microstructural embrittlement in the weld region which caused extensive secondary cracking along the interfaces of austenite/σ-phases and their coalescence, was more pronounced with an increase in the hold time and temperature. The variation in life was seen to be consistent with the severity of cracking under different testing conditions.

Keywords: Weld joint; Thermal ageing; Low cycle fatigue; Microstructural embrittlement; Fatigue-creep interaction.

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Investigation of Nanoscale Precipitation in 17-4PH Stainless Steel using Small-Angle Neutron Scattering

Gokulnath Kadavath[1, *], Yadunandan Das[2], Diego Alba Venero[3], Emily Aradi[4], Mohammed Kashif Khan[1], Michael E Fitzpatrick[1]

[1]*Faculty of Engineering, Environment & Computing, Coventry University, Coventry CV12JH, UK*

[2]*Engineering and Innovation, The Open University, Walton Hall, Milton Keynes, MK7 6AA, United Kingdom*

[3]*ISIS Pulsed Neutron and Muon Source, STFC Rutherford Appleton Laboratory, Harwell Campus, Didcot, OX11 0QX, United Kingdom*

[4]*Department of Engineering and Sustainability, University of Manchester, Manchester M13 9PL, United Kingdom*

*Corresponding Author E-mail: gokulnath@cet.ac.in

ABSTRACT

The evolution of nanoscale phase separation in the precipitation hardenable 17-4PH grade steel has been quantitatively investigated by small-angle neutron scattering (SANS) and electron microscopy. The results were correlated with atom probe tomography investigations by Yeli *et al.* [1] and *Wang et al.* [2] and were found to be in good agreement. The coarsening of the precipitate is related to the diffusion rate of copper in 17-4PH steel at a given temperature as well as the coalescence of elements such as chromium (Cr), nickel (Ni), and iron (Fe), during thermal ageing. The SANS data fitted using spherical and ellipsoidal models indicated the morphology change of Cu-rich precipitates with growth from BCC matrix to 9R ellipsoidal structure.

Keywords: Martensitic stainless steels; Precipitation hardening; Small-angle neutron scattering (SANS); Kinetics of precipitation.

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Synergistic Effluent Treatment through Adsorption and Photocatalysis using Banana Peel-Based ZnO Nanoparticle Composites

Simranjit Singh[1,2]**,** Vishakha Takhar[3], Himarati Mondal[2], Rupak Banerjee[3], Bhaskar Datta[2,4, *]

[1]*Department of Electronic System Engineering, Indian Institute of Science, Bangalore, Karnataka-560012, Karnataka, India*

[2]*Department of Chemistry, Indian Institute of Technology Gandhinagar, Palaj, Gandhinagar-382355, Gujarat, India.*

[3]*Department of Physics, Indian Institute of Technology Gandhinagar, Palaj, Gandhinagar-382355, Gujarat, India.*

[4]*Department of Biological Engineering, Indian Institute of Technology Gandhinagar, Palaj, Gandhinagar-382355, Gujarat, India.*

*Corresponding Author E-mail: bdatta@iitgn.ac.in

ABSTRACT

Composites combining biomass-derived materials with inorganic nanomaterials can synergize complementary adsorptive and redox-reactive properties of the constituents. In this work, we have synthesized an organic-inorganic composite combining dried and crushed banana peel (DCBP) with in situ generated ZnO nanoparticles, and assessed the ability of the composite to degrade Methylene Blue (MB) dye in comparison to pristine DCBP and ZnO. The composite exhibited an impressive 43% adsorption capacity of MB compared to 20% for DCBP and 1.5% for ZnO nanoparticles with 5 mg L^{-1} of MB. A 95% efficiency of degradation was observed for the composite with the highest kinetic rate of 03064± 0.006 min^{-1} under 60 mins of exposure time. The DCBP-ZnO composite was reusable across 5 cycles accompanied by a high 88% removal efficiency. The composite displayed high removal efficiencies on 84.3%, 47.7%, and 52%, for Eosin B, Rhodamine B and MB, when the dyes were combined. The composite resulted in significant degradation of real industrial effluent samples. The enhanced dye removal by the DCBP-ZnO was scrutinized by scavenger test that confirmed the formation of reactive oxygen species. The composite exhibits superior dye remediation by synergizing the distinctive adsorption characteristics of the biomass-constituent and the high photocatalytic efficiency of integrated ZnO nanoparticles.

Keywords: Organic-inorganic composites; Banana peel; ZnO nanoparticles; Photocatalysis; Effluent treatment.

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DFT-Driven Generation of ANN Potentials For 316LN Stainless Steel

P Surya Samyog, Jeetu S Babu*, and Telagathoti Suresh Kumar
[1]*Department of Materials Science and Engineering, National Institute of Technology, Calicut, NIT Campus PO, Kozhikode, 673601, Kerala, India*

*Corresponding Author E mail: jeetusbabu@nitc.ac.in

ABSTRACT

Traditional molecular dynamics (MD) simulations often rely on empirical potentials, which lack the accuracy to fully capture complex atomic interactions, limiting their predictive power. Ab-initio methods like DFT calculations are computationally expensive and hence cannot be solely relied on. To address this issue, we use DFT calculations to generate a reference dataset of structural and energy data to build an Artificial Neural Networks (ANN) model with an open-source package, net to develop the potential of ANN. Highly accurate ANN potentials can be used instead of empirical potentials to make MD simulations more accurate and reliable. Reference structures and energy data points of 316LN SS are generated using DFT calculations. The data is used to train a model with the help of ænet package, which generates accurate ANN potentials. These potentials can be integrated with MD simulations to measure the mechanical behaviour of the alloy. This project aims to build a reliable method to predict the ANN potentials of 316LN SS and study the mechanical behaviour which could serve as guidelines to future research and also help in manufacturing and materials selection.

Keywords: DFT; Python; ANN; ænet, molecular dynamics; Ab initio.

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Aerodynamic Investigation of Blended Wing Body

Resmi V Prasad*, Akash A S, Ambrose Antony, Nihal N, S D Vishal

Aeronautical Engineering, ACE College of Engineering, Thiruvallam, Trivandrum, India

*Corresponding Author E-mail: resmi.prasad@acetvm.com

ABSTRACT

A full-lifting surface aircraft with a blended wing body (BWB) configuration has wings and fuselage that are tightly melded together. Under a specific load requirement, the BWB architecture can decrease the wetted area of the entire aircraft, hence reducing frictional drag. The BWB configuration is 15%–20% more efficient at cruising than the conventional layout, and it also has the advantages of lessening structural weight and noise emissions, among other possible benefits. The BWB layout is practical for commercial transport aircraft due to these benefits. A BWD aircraft's aerodynamic performance can be increased in a number of ways, including by altering the wing shape, the engine layout, the sweep angle, and numerous other structural alterations. In this project, a BWB airplane designed in CATIA and ANSYS is printed in PLA as a prototype and subjected to experimental study in a subsonic wind tunnel. The main objective of this study was to identify the optimum BWB aircraft design that achieves a balance between high fuel efficiency, minimal interference drags, and noise reduction. By analysing the experimental data and evaluating the performance of different design configurations, valuable insights can be gained to inform future developments in BWB aircraft technology. The findings of this study contribute to the ongoing efforts in advancing the practicality and effectiveness of blended wing body aircraft for commercial transport purposes.

Keywords: Blended wing; Aerodynamics; Sweep angle; Drag.

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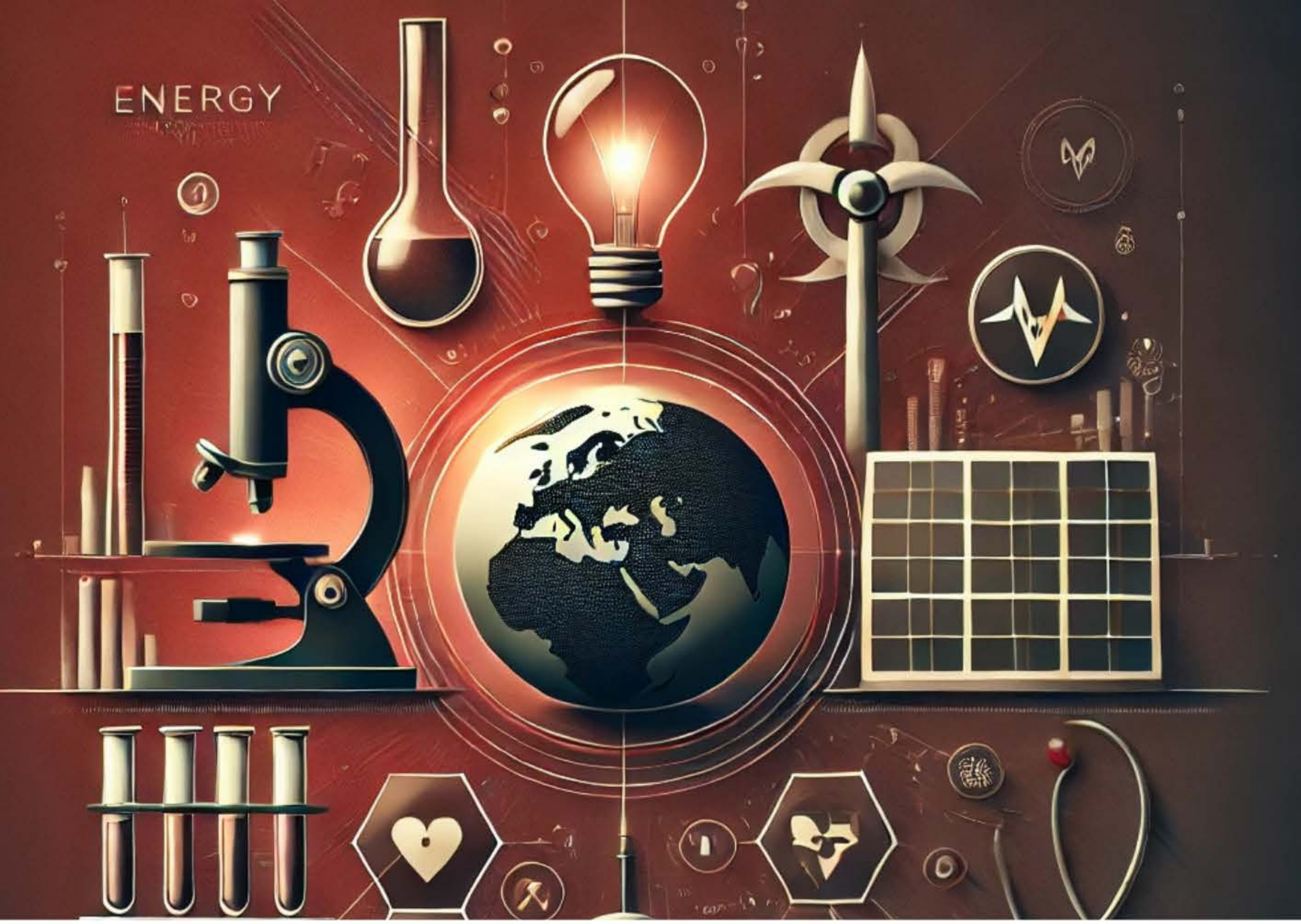

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