

Proceedings of

iCEAME International Conference
on Emerging Areas
in Materials Engineering

AICERA 2017

7th ANNUAL INTERNATIONAL CONFERENCE
ON EMERGING RESEARCH AREAS

13-15, July 2017



AMAL JYOTHI
COLLEGE OF ENGINEERING
KANJIRAPPALLY

Proceedings of

**International Conference on Emerging Areas in
Materials Engineering (ICEAME 2017)**

**7th Annual International Conference on
Emerging Research Areas (AICERA)**

13-15, July 2017



Amal Jyothi College of Engineering
Kanjirappally, Kerala, India

Foreword

It is with immense pride and joy we present the proceedings of the International Conference on Emerging Areas in Materials Engineering (ICEAME 2017), which is the seventh edition of the Annual International Conference on Emerging Research Areas (AICERA), organized by Amal Jyothi College of Engineering every year.

ICEAME-AICERA 2017 is being organized jointly by the Departments of Chemical Engineering, Metallurgy and Basic Sciences of the College, with focus on different aspects of Materials Science and Engineering. This area has been chosen as the theme of the conference this year because several faculty members of the college, particularly those in the above Departments, are active researchers in Materials Science and Engineering. Moreover, the College now offers an M. Tech. programme in Nanotechnology, which is very close to the focal theme of the conference. The organizing committee decided to cover the following specific track themes in materials science for the conference.

Smart Materials/ Biomaterials/ Shape Memory Alloys, Nanomaterials/ Novel Materials, Ferroelectric/ Multiferroic/ Electronic Materials, Ceramics/ Composites/ High Temperature Materials, Photonic/ Photovoltaic Materials, Low Dimensional Systems/ Carbon nanostructures/ Graphene, Thin Films/ Interfaces, Polymers/ Conducting Polymers/ Organic Materials, Superconductors/ Spintronic materials/ Magnetics, Environmental Issues/ Green Materials, Energy Harvesting Materials/ New Gen Materials, Materials Characterization/ Novel techniques, Computational methods/ Modeling.

During the three-day conference, the participants shall listen to engineers, academicians, scientists, industry researchers, research scholars and students from the fields of Material Science and Engineering, Metallurgy, Chemical Engineering, Physics, Chemistry and allied areas. The conference shall feature invited talks by experts in the respective fields, contributed lectures and poster presentations by younger researchers, focusing on specific current trends in the theme areas and shall discuss recent advances, challenges and breakthroughs in modern materials science and engineering. The organizing committee identified 14 experts to deliver invited talks. All the submitted contributed papers have been peer-reviewed and 40 of them have been finally selected for presentation at the conference.

We cordially invite all invited speakers and contributors to this part of Kerala and India where there are a good number of tourist attractions close by, like Munnar (best tourist spot in Asia based on UNESCO), Thekkady wild life Sanctuary, Wagamon hill station comprising of a series of beautiful hillocks, valleys and waterfalls, famous

backwaters of Kerala, beaches etc. We hope the participants shall enjoy their stay here at Kanjirappally.

I take this opportunity to thank each and every one of those who have contributed to the successful conduct of the conference. I thank the Management, Principal, Officers, Faculty, Staff and Students of the College for their whole-hearted support and cooperation. I particularly thank the Organizing Committee members, whose hard work has made this a reality.

Dr. J. Philip,
Convener, ICEAME-AICERA 2017,
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DISCOVERY OF NEW MATERIALS BY SIMULATION AND EXPERIMENT: FROM MOLECULAR RECOGNITION TO CATALYSTS, COMPOSITES, AND THERAPEUTICS

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The discovery of novel functional materials remains largely driven by tedious trial-and-error studies, whereby the rational understanding and design using modeling and simulation play an increased role thanks to more affordable computing resources. This talk introduces modeling techniques and their capabilities at the 1 to 1000 nanometer scale, describing molecular recognition mechanisms on metals, oxides, and biominerals (apatites). Applications to nanocrystal growth, catalyst design, composites, and therapeutics are shown. To support such applications, the mechanism of specific adsorption of polymers and biomacromolecules onto metallic and oxides nanostructures will be described in atomic detail resulting from simulations with novel force fields and surface models in comparison to measurements (Figure 1). Variations in peptide adsorption on Pd and Pt nanoparticles depending on shape, size, and location of peptides on specific bounding facets are determined by soft epitaxial processes and induced charges in solution. Accurate computational predictions of reaction rates in C-C coupling reactions using particle models derived from HE-XRD and PDF data illustrate the utility of computational methods for the rational design of new catalysts. On oxides nanoparticles such as silica and apatites, it is shown how

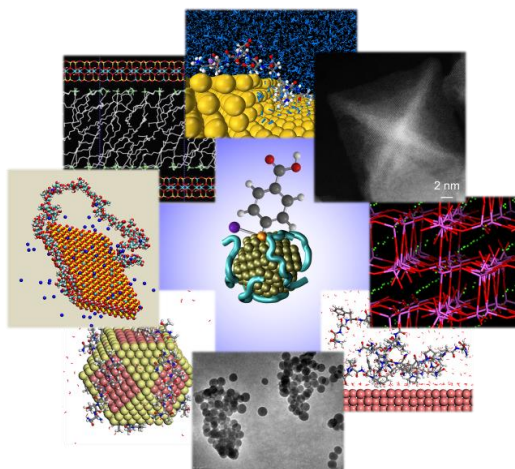


Figure 1: Examples of biomolecular recognition on inorganic surfaces and interfacial features that determine surface reactivity.

changes in pH lead to similarity scores of attracted peptides lower than 20%, supported by model surfaces of appropriate surface chemistry and data from adsorption isotherms. The results demonstrate how new computational methods can support the design of structured hydrogels, nanoparticle carriers for drug release, and the understanding of calcification mechanisms in the human body. Also, new insight into the interaction of polymer with carbon nanotubes for high strength carbon fibers along with relationship to shear strength and glass transition temperatures will be discussed. General theoretical foundations of accurate force fields (the INTERFACE force field) for simulations of inorganic/organic and inorganic/biological hybrid materials will be explained and illustrated at hand of examples.

References

1. H. Heinz and H. Ramezani-Dakhel. *Chem. Soc. Rev.* **45**, 412 (2016).
2. N. M. Bedford, H. Ramezani-Dakhel, J. M. Slocik, B. D. Briggs, Y. Ren, A. I. Frenkel, V. Petkov, H. Heinz, R. R. Naik, and M. R. Knecht. *ACS Nano* **9**, 5082 (2015).
3. H. Heinz, T. J. Lin, R. K. Mishra, F. S. Emami. *Langmuir* **29**, 1754 (2013).

Invited Talk 2

ADVANCES IN MATERIALS AND THE ROLE ON PERFORMANCE IMPROVEMENT POWER GENERATION SYSTEMS

Dr. Bale V. Reddy

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The global energy demand is growing and this has to be met through development of efficient and advanced energy systems and through various energy conservation measures. The advances and developments in the field of materials and processes are helping in better design of turbine blades, thermal and power generation systems. This has influence on efficiency of thermal and power generation systems. The presentation will focus on the developments and advances in the material field, the development of blade materials and the related developments in steam cycle, gas cycle, combined cycle power generation, solar and wind power generation systems. The role of second law of thermodynamics on the performance improvement of thermal and power generation systems with advances in materials will be presented. The exergy analysis for power generation systems and its role on plant performance improvement will also be discussed.

Invited Talk 3

2D MATERIALS BEYOND GRAPHENE: CONTROLLABLE SYNTHESIS AND APPLICATIONS

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The discovery of graphene has opened up new horizons in material science research, with its unique and spectacular physical, mechanical, electrical and optical properties.¹ Graphene research has sparked great interest in a wide range of 2-dimensional layered materials with varying electronic properties. Atomically thin layered transition metal dichalcogenides (TMDs) such as MoS₂, WS₂, MoSe₂ and WSe₂ have been emerging as the cutting edge in materials science and engineering, due to their interesting electronic properties.² These materials open up new opportunities for a variety of applications, including optoelectronics, energy conversion, and catalysis. To realize their potential device applications, it is highly desirable to achieve controllable growth of these layered nanomaterials, with tunable structure and morphology.³⁻⁶ In this talk, I will first introduce the controlled synthesis technique that we have recently developed for the growth of luminescent quantum dots of TMDs.⁶ Such tailored materials show exceptional electrocatalytic properties towards hydrogen evolution reaction (HER). The talk will also present some of our recent efforts on morphological and optical studies of chemical vapour deposition (CVD) grown spiral and pyramid-like few-layer TMDs.

References

1. A. K. Geim, K. S. Novoselov, *Nat. Mater.* **2007**, 6, 183-191.
2. H. R. Gutiérrez, N. Perea-López, A. L. Elías, A. Berkdemir, B. Wang, R. Lv, F. López-Urías, V. H. Crespi, H. Terrones, M. Terrones, *Nano Lett.* **2013**, 13 (8), 3447-3454.
3. Y. Gong, P. M. Ajayan et al., *Nat. Mater.*, **2014**, 13, 1135-1142
4. D. Gopalakrishnan, D. Damien and M. M. Shaijumon, *ACS Nano*, **2014**, 8, 5297-5303.
5. D. Damien, A. Anil, D. Chatterjee and M. M. Shaijumon, *J. Mater. Chem. A* (**2017**), DOI: 10.1039/c6a09645j
6. D. Gopalakrishnan, D. Damien, B. Li, H. Gullappalli, V. K. Pillai, P. M. Ajayan, and M. M. Shaijumon, *Chem. Commun.* **2015**, 51, 6293-6296

Keywords: Magnetic Tunnel Junctions; SGGA; bandstructure; TMR; Co/MgO/Co; magnetization

Invited Talk 4

**A NOVEL BIOMOLECULE MEDIATED SYNTHESIS OF GRAPHENE
OXIDE-SILVER NANOPARTICLE NANOCOMPOSITE: A POTENTIAL
ANTICANCER NANOTHERAPY**

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Graphene has been extensively used for cancer therapy because of its unique properties. The use of graphene to target and eliminate cancer stem cells (CSCs) is an alternative approach to conventional chemotherapy. CSCs are able to survive conventional chemotherapy. Thus, there is an urgent need for novel approaches to cancer therapy. In this study, biomolecule-mediated reduced graphene oxide-silver nanoparticle nanocomposites (rGO-Ag) were synthesized using c-phycocyanin (CP) as a reducing and stabilizing agent. The anticancer properties of CP-rGO-Ag were evaluated in human ovarian cancer cells. The synthesized CP-rGO-Ag nanocomposite was characterized using various analytical techniques. The anticancer properties of the CP-rGO-Ag nanocomposite were evaluated using a series of cellular assays and clonogenic assay. The expression of apoptotic and anti-apoptotic genes was measured by real time quantitative reverse transcriptase polymerase chain reaction (qRT-PCR). The prepared CP-rGO-Ag nanocomposite showed significantly greater cytotoxicity towards ovarian cancer cells than graphene oxide, reduced graphene, and oxide and silver nanoparticles. Further, the toxicity of the CP-rGO-Ag nanocomposite was due to a loss of mitochondrial membrane integrity and enhanced expression of apoptotic genes, leading to adverse changes in the mitochondrial function and possibly triggering apoptosis. The prepared CP-rGO-Ag nanocomposite showed significant cytotoxic potential in human ovarian cancer cells. These findings suggest that CP-rGO-Ag could be a novel nanotherapeutic molecule for the specific targeting and elimination of CSCs.

Keywords: Graphene, silver nanoparticles; anticancer; nanomedicine; nanotherapy

Invited Talk 5

AMORPHOUS OXIDE THIN FILM TRANSISTORS FOR THE APPLICATION OF TRANSPARENT FLEXIBLE ELECTRONICS

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Amorphous oxide semiconductors (AOS) have attained considerable attention for the past few years because they are the potential materials for replacing some of silicon based microelectronic devices such as flat panel displays. The major advantage of oxide semiconductor materials over silicon is that they can be deposited uniformly over large area at low temperature. The low temperature deposition of AOS on flexible plastic substrates using conventional methods like sputtering enables a new area of research called transparent flexible electronics.

The development of AOS thin film transistors, which is a key component of display units, are excellent candidates for switching or driving transistors in next generation active matrix liquid crystal displays (AMLCD) or active matrix organic light emitting diode (AMOLED) displays. For the past few years researchers are working on AOS TFTs mainly focusing on the major issues like stability of TFTs in order to move from basic research to product generation. However in comparison with organic thin film transistors (OTFTs), which also can deposit on flexible substrates, the AOS TFTs have high mobility and environmental stability. At present indium gallium zinc oxide, zinc tin oxide, zinc indium oxide, zinc indium tin oxide etc are the most used channel materials for the fabrication of AOS based TFTs. Indium free systems are highly preferred for their cost effectiveness. Hence among the above mentioned materials zinc tin oxide (ZTO) is more favourable and economical for fabricating high performance TFT. The high performance of the ZTO TFTs enables the realization of dynamic circuits like inverters and ring oscillators. Display companies are now very close to reaching mass production of AOS based commercial products like flat panel display, sensors, wearable devices like watches etc. Moreover, the fundamental research on the mechanisms that govern device stability and ways to overcome those limitations may lead to replacement of Si technology by AOS technology in near future. In this paper, the fabrication of n-channel ZTO and p-channel CuO TFTs will be discussed. These have been successfully integrated to form CMOS inverter.

References

1. E. Fortunato, P. Barquinha, and R. Martins, Adv. Mater. 24, 2945 (2012).
2. J.S. Park, H. Kim, and I.D. Kim, J. Electroceramics 32, 117 (2014).
3. H.Q. Chiang, J.F. Wager, R.L. Hoffman, J. Jeong, and D.A. Keszler, Appl. Phys. Lett. 86, 013503 (2005).

Invited Talk 6

**ULTRAFAST LASER INDUCED PERIODIC SURFACE STRUCTURING
(FS-LIPSS) AND APPLICATIONS**

Reji Philip

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Surface morphology is a key factor in controlling the optical, mechanical, wetting, chemical, and biological properties of solid surfaces. Femtosecond laser induced surface structuring (fs-LIPSS) has emerged as a novel and versatile technology for producing a large variety of micro and nanostructured materials, suitable for a wide range of applications in photonics and materials science. In LIPSS, a regular groove structure will be formed on the target surface with a period of the order of the laser wavelength, oriented perpendicular to the polarization of the incident light. The groove period on the material surface can be controlled by changing the laser parameters, target material, and ambient conditions. Even though many technological improvements have been made in this area, the physical mechanisms of LIPSS, precise control of groove period, and complex pattern formation are still being studied by many investigators. We are presently working towards predictable control of the period of LIPSS by controlling laser parameters (wavelength, pulse duration, fluence, and orbital angular momentum) and ambient conditions. The fundamental principles of LIPSS and its various applications will be discussed in this talk.

Invited Talk 7

**IMPACT OF NANOTEXTURING ON HIGH PERFORMANCE GAN-BASED
LIGHT EMITTING DIODES**

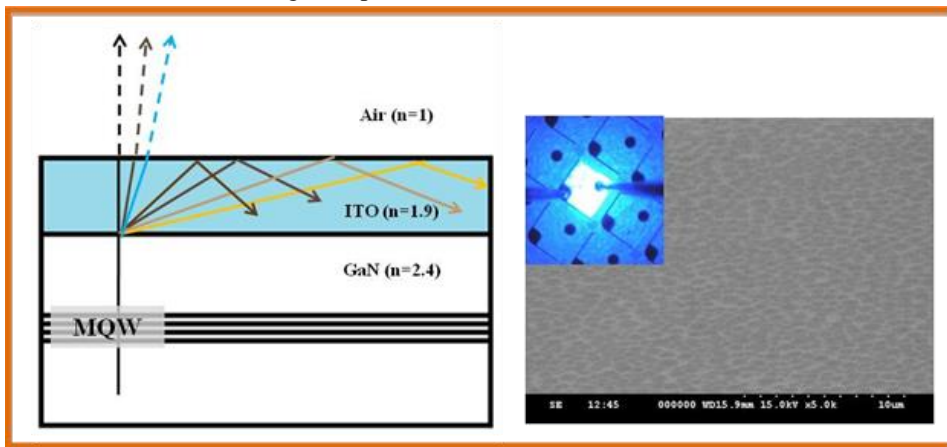
Dr. A.P. Uthirakumar

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The fabrication of high performance gallium nitride-based light emitting diodes (GaN-LEDs) is a major anxiety for next generation electronics. The prime limitation is external quantum efficiency is limited by the total internal reflection, and the angle of the light-escape cone is very small due to a large difference in the refractive index between the semiconductor and air interface. As a result, intense work has to be focused on an improvement of the external quantum efficiency of the device. Several approaches, including surface texturing on the p-type electrodes are one of the effective methods for improving LED efficiency. Here, we have demonstrated nanotexturing technique to improve the output power of LEDs by 25-30%, when compared to conventional flat LEDs.. Figures show the simulation and SEM image of nanotexturing impact to enhance the high performance of GaN-based LEDs. Although few other techniques have yielded positive results,

the complex and expensive processing along the incurred surface damage are significant barriers for the device fabrication at high temperature.



Invited Talk 8

TEMPERATURE DEPENDENT PROPERTIES OF Mn:ZnS NANOPARTICLES

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X-ray diffraction (XRD), Ultraviolet-visible (UV-vis), Photoluminescence (PL) and Electron paramagnetic resonance (EPR) spectroscopy techniques are used for structural analysis of Mn doped ZnS nanoparticles at different temperatures. XRD analysis confirms the nanostructure of the sample with 4-15 nm of average crystallite size. As temperature increases size of the particles are also increases. UV-vis absorption spectra show blue shift as compared to bulk ZnS. EPR shows the existence of Mn^{2+} with different local structures in ZnS nanoparticles. The values of spectroscopic splitting factor (g) and hyperfine interaction constant (A) decrease as Mn^{2+} concentration increases in ZnS Nanoparticles as well as increase in temperature. The photoconductivity behavior of Mn doped ZnS nanoparticles are also studied at different temperatures. It is observed that on increasing the temperature of the samples, photoconductivity increases.

Invited Talk 9

NANO GRAIN FERRITE THIN FILMS – AN EFFECTIVE WAY TO TUNE IN DESIRABLE MAGNETIC & TRANSPORT PROPERTIES IN SPACE CONSTRAINED MINIATURE ELECTRONIC GADGET ARCHITECTURE**Dr. Jaison Joseph***Associate Professor & HOD, Dept. of Physics, Govt. College. Khandola. Marcela. Goa.*

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Spinel Ferrites are a class of oxide materials effectively used in the manufacture of electronic components installed in devices such as mobile phones and tablets for signal detection. These types of materials also find exclusive industrial usage in bulk manufacture of device components such as transformer cores, audio and video recording heads, rod antennas, memory devices, and radio frequency coils, which are widely used in various electronic gadgets. Presently there exists an impressive research effort to miniaturize electronic components in line with the principle of reducing gadget dimensions. To facilitate this industry, desirable ferrite oxide materials are to be produced in thin film form with critical film thickness which entirely depends on its applicable space available in the gadget architecture.

In a recently accomplished research endeavor, novel ferrite thin films were fabricated on a Pulsed Laser Depositor (PLD) and Radio Frequency (RF) sputtering deposition system using nano ferrite materials synthesized by us. Investigations into the structural details of thin films fabricated by RF sputtering technique revealed creation of pure c-axis grown nano grain ferrite films at a critical low film thickness. The ferrite thin films fabricated by PLD showed novelty by enhanced texture, nano grain dimensions and moderate film thickness. Measurements of magnetic parameters of these thin films using Superconducting Quantum Interface Device (SQUID) VSM resulted in an observation of enrichment in industry desirable magnetic properties. An improvement in desirable electric properties were also observed in these thin films by performing experiments on a four probe thin film resistance measurement system specially designed, developed and fabricated for thin film resistance measurements.

The industry favorable improvements in electric and magnetic properties observed in these thin films provide an effective modus operandi which can be adopted in component manufacture where in ferrite materials are utilized under stringent space control. This attains peak significance in miniature electronic component manufacture where in the utilizations are at space constrained environments such as satellites or defence electronic equipments. Scientific explanations for these improvements in desirable properties were also derived by proposing an appropriate film growth model.

Invited Talk 10

COARSE-GRAINED MODELS FOR POLYMERS – UNDERSTANDING OF POLYMER STRUCTURES AND INTERACTIONS WITH SOLVENTS

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Smart polymeric systems are being designed for various novel applications. These polymers are expected to have one or more of the following characteristics, conductivity, electromechanical response, volume phase transition, etc. We have been using Coarse-grained models to derive fundamental understanding of polymers involved in the following two examples. In this talk, we will summarize the questions posed, methods used, and the deductions from modeling.

The mechanism of the lower critical solution temperature (LCST) in thermoresponsive polymer solutions has been studied by means of a coarse-grained single polymer chain simulation and a theoretical approach. The results of this study indicate that the LCST behavior is determined by the competition between the mean energy difference between the bulk and bound solvent, and the entropy loss due to the bound solvent [1].

In particular, a structure-based systematic coarse-graining approach was adopted to coarse-grain sulfonated poly(ether-ether-ketone), sPEEK, an emerging candidate as a proton exchange membrane (PEM) for application in fuel cells, to enable rheological studies on the water channels in sPEEK membranes. The methodology was subsequently used to investigate the effect of hydration on sPEEK membranes [2,3].

References

1. Bharadwaj S., Kumar P. B. S., Komura S., Deshpande A. P., Spherically Symmetric Solvent is Sufficient to Explain the LCST Mechanism in Polymer Solutions, *Macromolecular Theory and Simulations*, DOI: 10.1002/mats.201600073.
2. Tripathy M., Deshpande A. P., P. B. Sunil Kumar, How much can we coarse-grain while retaining the chemical specificity? A study of Sulfonated Poly(ether ether ketone), *Macromolecular Theory and Simulations*, 25 (2), 155-169 (2016).
3. Madhusmita Tripathy, Sunil Kumar P. B., Abhijit P. Deshpande, Molecular Structuring and Percolation Transition in Hydrated Sulfonated Poly(ether ether ketone) Membranes, *Journal of Physical Chemistry B*, under review.

Invited Talk 11

RECENT DEVELOPMENTS IN RUBBER NANOCOMPOSITES

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Nano-dispersions and emulsions have got wide acceptance in rubber industry. High activity, good transparency, less environmental issues are the added advantages of these materials. It has been reported that nano-dispersions can offer remarkable improvements in the adhesive properties. The solvent based conventional adhesives can be completely replaced by water based adhesives with suitable nano-additives. Polymer nanocomposites reinforced by relatively small amounts of ultra-fine, nano-particles (most often clay platelets) proved exceptionally promising engineering materials with unexpectedly high stiffness/toughness ratio, gas barrier properties, flame retardance, etc.

Graphene related materials such as exfoliated grapheme oxide and reduced grapheme oxide recently achieved much interest in nanocomposite research. Polymer grapheme nano-composites showed excellent conductivity at lower percolation threshold. Addition of rubber chemicals as fine particle dispersions in latex technology will improve the product clarity and also will reduce the rejection rates in thin walled products like gloves, condoms etc. Large abundance, low cost and eco-friendliness of bio-materials such as starch, cellulose, chitin etc., need to explore their suitability as alternative candidates for conventional inorganic fillers in rubber industry. The bio-degradable nature of these materials offers several other advantages also.

The study is focused on the different methods used for the preparation of nano-dispersions and their applications in the rubber industry, electronics etc.

Invited Talk 12

TRANSPORT PROPERTIES OF QUANTUM ONE-DIMENSIONAL CONDUCTORS

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Transport in one-dimensional devices has attracted wide interest since the discovery of conductance quantization in a short one-dimensional ballistic constriction defined in a GaAs/AlGaAs heterostructure in 1988. Interest has since grown steadily, mainly due to several theoretical predictions of novel effects due to Coulomb interactions in one-dimension. In this talk, I shall present experimental evidence of spin-related transport in quantum wires. Starting with the discovery of an additional conductance structure at $0.7(2e^2/h)$ called the 0.7 structure [1] in

ballistic quantum wires, a many body spin effect, experimental evidence for a fully spin polarized state achieved by manipulating the symmetry of the potential confinement using a scanning gate techniques will be presented. Several theoretical models were proposed to explain the 0.7 structure including spin polarization, Kondo effect, spin-incoherent transport, and Wigner crystallization. Recent experimental results from quantum wires fabricated with an additional top gate to examine the effect of confinement strength and density show that spin waves are reflected in a certain energy range, giving rise to a structure at e^2/h due to spin-incoherent transport. Understanding transport mechanisms that involve spin of the electron are significant. Here I present experimental data of semiconductor nanostructure devices where spin-related transport is observed.

References

1. K. J. Thomas, J. T. Nicholls, M. Y. Simmons, M. Pepper, D. R. Mace, and D. A. Ritchie. "Possible Spin Polarization in a One-Dimensional Electron Gas", Phys. Rev. Lett. 77,135 (1996).
2. R Crook, J. Prance, K. J. Thomas, S. J. Chorley, I. Farrer, D. A. Ritchie, M. Pepper, and C. G. Smith. "Conductance quantization at a half-integer plateau in a symmetric GaAs quantum wire" Science 312, 1359 (2006).
3. W. K. Hew, K. J. Thomas, M. Pepper, I. Farrer, D. Anderson, G. A. C. Jones, and D. A. Ritchie, "Spin-incoherent transport in quantum wires" Phys. Rev. Lett., 101, 036801 (2008).

Invited Talk 13

TEMPLATE ASSISTED FABRICATION OF 1-D MAGNETIC NANOSTRUCTURES FOR APPLICATIONS

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Engineering materials for various applications requires specific process control parameters. With the advent of nanotechnology, tuning the size and shape of materials results in superlative properties. Though various methods for fabrication of 1-D nanomaterials exist, template assisted electro deposition is a sought after method. However, precise fabrication of magnetic nanostructures requires proper understanding of the mechanism of formation of these nanostructures. The method of template assisted deposition was utilized to fabricate magnetic nanostructures of Co, Ni, Carbon Nano tube –Co. They were characterized using various analytical tools. The template used was alumina. The mechanism of formation of these nanostructures was elucidated and this knowledge was utilized to create core-shell architectures to suit different applications. Application potential of these structures are demonstrated. Finally, a magneto-electric coupled device was fabricated. The details will be discussed here.

References

1. Synthesis of high coercivity cobalt nanotubes and elucidation of their mechanism of growth, J. Phys. Chem. C., 112 (2008), 14281-14285

2. The synthesis of high coercivity cobalt in carbon nanotube heterostructures and their optical limiting properties, *Nanotechnology* (2009), 20.285702
3. Synthesis of high coercivity core-shell nanorods based on Nickel and cobalt and their magnetic properties, *Nanoscale Res. Lett.* (2009)1.007/s1671-009-9459-7
4. Template assisted synthesis and characterization of passivated nickel nanoparticles, *Nanoscale Res Lett.* (2010); 5(5): 889–897

O1.1

CHARACTERIZATION OF FINE PRECIPITATES EVOLUTION IN POST AGEING TREATMENT AFTER FRICTION STIR PROCESSED 7075 AL ALLOY

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The effect of post ageing temperature (140°C for 2h) on the microstructure and mechanical behaviour of FSPed 7075 Al alloy has been studied by optical microscopy (OM), field emission scanning electron microscopy (FESEM), scanning electron microscopy (SEM), differential scanning calorimetry (DSC), transmission electron microscopy (TEM), and mechanical properties. Friction stir processing (FSP) is a solid state surface modification technique to apply for cast aluminium alloy. FSP has a similar metal working principle like FSW (friction stir welding). Despite, strong age-hardening response with Sc (scandium) inoculated Al-Zn-Mg alloy, because of the novelty of FSP only few studies have been carried out on the effect of post ageing treatment on the microstructure, size, morphology and fine dispersion of coherent Al₃Sc (L1₂ type) precipitates or η -phases (MgZn₂) and mechanical properties of FSPed 7075 Al alloy. The FSP enhances grain boundary (GB) formation and increases suitable sites for the precipitation of nucleation in post aged 7075 Al alloy. The experimental mechanical properties have been evaluated such as proof strength ($\sigma_{0.2}$) of 122.9 MPa, ultimate tensile strength (σ_u) of 256.4 MPa, ductility (δ) of 8.6%, Vicker's hardness (along the stir zone) of 101 HV, and strain hardening exponent (n) of 1.82, respectively.

Keywords: 7075 Al-alloy, TEM, Al₃Sc and η precipitates, mechanical properties.

O1.2

PREPARATION AND CHARACTERIZATION OF SUPERHYDROPHOBIC AND SUPEROLEOPHILIC POLYMER-COMPOSITE COATINGS FOR OIL-WATER SEPARATION APPLICATION

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Environmental pollution caused by industrial oily waste-water and oil-spill accidents, affects marine life and unbalances the ecosystem. Therefore, generation of efficient and reusable superhydrophobic (water contact angle $\geq 150^\circ$ and sliding angle $\leq 10^\circ$) and superoleophilic (oil contact angle $\sim 0^\circ$) polymer-composite coatings for oil-water separation is sought after. Naturally

occurring surfaces like lotus-leaf, butterfly wings, water-strider legs etc. have always inspired material scientists to mimic its surface structure, properties and geometry for development of superhydrophobic and superoleophilic coatings. Superhydrophobic coatings have widespread applications in automobiles, textiles, electronic devices, industries etc. which along with superhydrophobic property possess self-cleaning, anti-corrosion, anti-icing, anti-fogging and oil-water separation properties. In the current work, porous superhydrophobic and superoleophilic linear low density polyethylene (LLDPE) and silica (SiO_2) nanoparticles embedded LLDPE coatings on filter paper were fabricated using solution-casting technique. Surface morphology, water contact angle, and chemical composition of uncoated and coated filter papers were investigated. SiO_2 nanoparticles embedded LLDPE coating on filter paper shows the maximum water contact angle of $167.8 \pm 1.4^\circ$ and sliding angle of $3.8 \pm 0.5^\circ$. Water-drop impact dynamics on the superhydrophobic coatings were also studied. Efficiency and reusability of coated filter papers to remove petroleum ether and benzene from oil-water mixture were also examined.

Keywords: Superhydrophobic; Superoleophilic; Polymer Coatings; Oil-water Separation

O1.3

DEVELOPMENT OF SUPER HYDROPHOBIC SPONGE FOR OIL SPILL SEPARATION

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With the growth of offshore oil exploration, production, and transportation, oil spills and other accidental pollution have become one of the most serious environmental and ecological problems. Oil spillage and the organic solvents discharged by chemical industries are primary pollutants of water resources, and have resulted in significant energy losses, serious environmental pollution and consequent ecological problems. Cleaning up oil spills and oil slicks from the surfaces of water and along the coastline, among other areas, is a challenging task. This research focus on the issue of developing super hydrophobic grapheme based melamine sponge with excellent oil sorption capacity and exceptional recyclability. Hydrophobicity will be measured in terms of contact angle. Sorption capacity of the newly developed sponge will be conducted in different organic solvents. Later an experimental set up will be developed to separate pure water from oil-water mixture by inducing super hydrophobicity in the melamine sponge.

Keywords: melamine sponge, superhydrophoby, contact angle, oil spills

O1.4

ENGINEERING NANOSTRUCTURED POLYMER BLENDS FOR EMI SHIELDING APPLICATIONS

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Precise control in dispersing nanofillers in a polymer blend is a key requirement in designing materials with tailored properties. In this study Electromagnetic Interference Shielding (EMI) materials were fabricated using PP/NR blends. In order to design materials which can shield electromagnetic radiations the electrical conductivity was targeted here using a conducting inclusion, MWCNTs. Interestingly the bulk electrical conductivity of the blend was enhanced due to the improved dispersion of MWCNTs. A significant enhancement in shielding effectiveness is also observed for the composites with different amount of MWCNT. Control over the precise location of nanoparticle is request to obtain better materials. It is shown here that localization of nanoparticles in the blend structure can result in excellent dielectric behaviour and electrical conductivity. Localization of nanoparticles in the blends can be monitored by TEM images. Phase morphology of the composites can be assessed using Scanning Electron Microscopy. This work opens up new paradigm for electromagnetic shielding applications with the aid of a sustainable and simplified method also.

Keywords: MWCNTs, Localization, EMI shielding

O1.5

MECHANICAL AND THERMAL PROPERTIES OF RGO AND GNP REINFORCED FKM NANOCOMPOSITES

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Fluoroelastomer (FKM) is a class of synthetic rubber with service life above 200°C with extraordinary levels of resistance to chemicals, oil and heat. FKM based composites are widely accepted in automotive, chemical and aerospace areas. In this study, FKM was reinforced with graphene derivatives by simple two-roll mixing technique. Nanocomposites were prepared from graphite nanoplatelets (GNPs) and microwave reduced graphene oxide (rGO). The filler materials

and the nanocomposites were characterized by FTIR-spectroscopy, X-Ray Diffraction technique and Raman spectroscopy studies. The developed FKM nanocomposites were analyzed for its effect on mechanical and thermal properties with filler loading. rGO reinforced FKM nanocomposites showed enhanced mechanical and thermal properties with lower filler loading compared to GNP reinforced FKM nanocomposites. For rGO/FKM nanocomposites optimum tensile properties were obtained with 0.75 phr of filler loading on the other hand with GNP, 8 phr loaded nanocomposite showed optimum mechanical properties. FKM/rGO with 0.75 phr of reinforcing content showed a tensile strength of about 5.793 MPa which is about 37% more than the gum sample. But the same result was obtained for GNP reinforced nanocomposite with 8 phr of filler loading. The thermal characteristic is also found to be pronounced for rGO reinforced nanocomposites compared to GNP nanocomposites. Increase in both the mechanical and thermal properties of the rGO nanocomposite with 0.75 phr filler loading is due to the proper dispersion of rGO in the nanocomposites which facilitates the transfer of stress uniformly through the matrix material and the thermal stabilities of the rGO filler component has been imparted to the nanocomposites respectively.

O1.6

**ELECTRICAL AND MAGNETIC PROPERTIES OF Er-DOPED
NANOPARTICLE DILUTE MAGNETIC SEMICONDUCTOR (DMS)
MATERIALS**

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Nanoparticles of Er-doped ZnO with general formula $Zn_{1-x}Er_xO$ ($x=0.02, 0.04, 0.05, 0.06, 0.08, 0.10$) were prepared by auto-combustion method using environment friendly fuel. XRD studies confirmed formation of nanoparticle hexagonal wurtzite structure for all samples with minor traces of Erbium oxide (Er_2O_3) in some materials. The average crystallite size in the range of 20 nm to 50 nm was obtained using Scherer's formula by applying corrections from Williamson's hall plots. SEM micrographs of the samples also indicated formation of nanoparticle samples. FTIR spectra of the prepared samples showed broad absorption peaks in the range of 390 cm^{-1} to 580 cm^{-1} in agreement with the reported results. Calculation of optical band gap from UV absorption spectra showed marginal decrease in the band gap with increase in Er concentration. Temperature-dependent resistivity profiles showed broad plateau regions between the temperature range of 50°C to 205°C for all the six samples showing no enhancement of phonon vibrations in the materials at these temperatures. However, a unusual peaking behaviour similar to phonon resonance peaks in the temperature range of 220°C to about 300°C followed by rapid fall in the resistivity was the general trend observed for all the samples. Temperature dependent thermo power synonymous to p-type at lower temperatures followed by a n-type at higher temperatures

was observed for these nanomaterials. Dielectric constant and dielectric loss versus frequency and temperature for all the samples was also studied. Magnetic measurements carried out using vibrating sample magnetometer (VSM) exhibited paramagnetic nature for all the DMS samples.

Keywords: Dilute magnetic semiconductor, rare earth, nanoparticles.

O1.7

TRADE-OFFS IN DIELECTRIC SPECTROSCOPY USING CAVITY PERTURBATION AT THE X-BAND

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Microwave cavity perturbation is a popular material characterization technique for measuring the complex relative permittivity of low loss materials. The method can be utilized in measuring the dispersion or the dielectric properties as a function of frequency, hence the name dielectric spectroscopy. Cavity perturbation is an accurate, but sensitive method requiring the perturbation to be just enough, meaning that the perturbation neither be too high to make the calculation complex nor be too low to make the frequency shift and Q-factor reduction insignificant. In addition, the accuracy of cavity perturbation measurement is (i) Material dependent - volume of the sample relative to that of the cavity, relative permittivity of the sample compared to air and (ii) Cavity dependent - mode of operation, the axis of perturbation, size and shape of the coupling hole and the slot for sample insertion. In the present paper, a rectangular cavity resonator is analyzed in a systematic manner using ANSYS HFSS, starting from the eigen modes of a simple rectangular cavity model to the resonant peaks of the complete cavity model typically used in experiments. Dielectric measurement using both the eigen mode perturbation and the resonant peak perturbation are also performed and compared for various TE-modes. Effects of various sample and cavity parameters on the dielectric properties are studied and trade-off factors are deduced. Some of the simulation results are validated using experiments using X-band cavity and VNA.

Keywords: Cavity perturbation, Rectangular cavity resonator, X-band, Complex permittivity

O2.1

AN ECO-FRIENDLY SYNTHESIS OF SILVER NANOPARTICLES USING AN INVASIVE AQUATIC WEED: *LIMNOCHARIS FLAVA*

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Green synthesis of silver nanoparticles (AgNPs) is one of the eco friendly and benign methods in the field of nanotechnology. In this study, solar energy has been utilized for the fast reduction of silver ions in to AgNPs using the otherwise worthless weed, *Limnocharis flava* (L.) Buchenau as a reducing as well as capping agent for the silver ions. When silver nitrate (AgNO_3) was mixed with an appropriate proportion of plant extract, the formation of AgNPs was observed by change in colour from green to brown which has grown intense within 30 minutes of irradiation. This is due to the phenomenon called surface Plasmon resonance. The nanoparticles were characterised using UV-Vis spectroscopy, Transmission Electron Microscopy (TEM), Fourier Transform infrared microscopy (FT-IR) and Atomic Force microscopy (AFM). Phytochemical analysis showed the presence of phenolics, Flavanoids, tannins and carbohydrates. The TEM micrograph reveals the presence of polydispersed spherical shaped nanoparticles in size from 30 to 120 nm. The presence of silver atom was confirmed by the EDAX. FT-IR spectra indicated the possible role of different functional groups in the plant extract for the reduction of silver ions in to AgNPs.

Keywords: Green synthesis, weed management, silver nanoparticles.

O2.2

STUDY ON SOLDERING OF SIMILAR AND DISSIMILAR ALUMINIUM ALLOYS USING ACTIVE SOLDERS

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Active soldering is an emerging technology of joining a range of materials, which utilizes Sn-Ag composition solder alloy other than conventional Sn-Pb solder, along with reactive element additions (e.g; Ti, Hf, Zr, and Ta). In the present study, active soldering is employed for bonding similar and dissimilar aluminium alloys using S Bond 220-50 active solder alloy. For this, AA 2014 and AA 7075 were selected for bonding. After soldering, mechanical properties were

evaluated using hardness and lap shear test. Microstructure analysis was carried out by optical and SEM microscopy. The soldered area was examined using EDS giving fair idea regarding the composition of elements present in the solder. It was observed that bonding of dissimilar aluminium alloys (AA 2014 soldered with AA 7075) showed better bond strength when compared with similar combinations of aluminium alloys and hardness was better in similar aluminium alloys. (AA 2014 soldered with AA 2014). The content of Ag dissolved in solder matrix and the role of Ti in forming reaction at solder-metal interface has influenced both bonding strength and hardness value.

Keywords: Active soldering, Sn-Ag solder, Sn-Pb solder, S Bond 220-50 solder alloy

O2.3

SYNTHESIS AND CHARACTERIZATION OF NANOSTRUCTURED PIEZOELECTRIC SODIUM POTASSIUM BISMUTH TITANATES WITH MORPHOTROPIC PHASE BOUNDARY

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Piezoceramic materials have been in commercial use for a long period. Owing to successful transfer of multilayer capacitor technology to the manufacture of multilayer actuators, their applications have multiplied over the last few decades. A large body of work has appeared in literature on the development of lead-free piezoceramics in a quest to replace Lead Zirconate Titanate (PZT) as the prime material for electro-mechanical devices such as actuators, sensors, and transducers. In specific application ranges, new lead-free materials appear adequate, but are not yet suited to replace PZT on a broad basis. This paper presents a novel method for the synthesis of nanostructured Sodium Potassium Bismuth Titanate (NKBT) and inducing Morphological Phase Boundary (MPB) structure in to it. This material is proposed as a potential one for the eventual replacement of PZT. KBT and NBT nanopowders are prepared separately following hydrothermal method and their solid solutions produced in different stoichiometric proportions to arrive at the MPB structure. X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM) are utilized to characterize the structure and morphology of the samples. Thermal, dielectric and piezoelectric properties of the samples have been measured and their piezoelectric figures of merit determined. It is found that the composition with MPB structure has high dielectric constant and piezoelectric figure of merit comparable PZT as well as other Bismuth Titanate based Aurivillius structures.

Keywords: Piezoceramics, Sodium Potassium Bismuth Titanate, Lead Zirconate Titanate, Piezoelectric properties, Dielectric properties

O2.4

ROLE OF SPIN-ORBIT INTERACTION ON ELECTRONIC PROPERTIES OF Cu BASED TERNARY ZINTL PHASES

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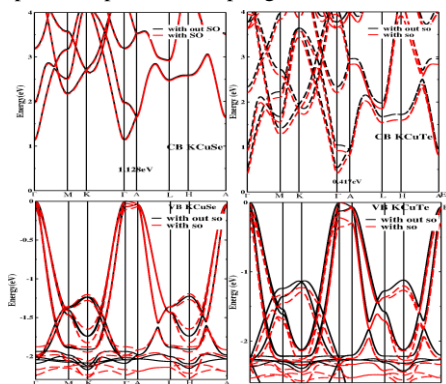
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The narrow band-gap semiconductors have been of great interest for the last four decades for their fundamental physics and their application in infrared devices, LEDs, infrared lasers and thermophotovoltaics [1]. In particular, copper-based systems with ternary direct band gap semiconductors are of great interest because of their potential application as thermoelectric components, thin-film photovoltaic (PV) absorbers, solar cell absorbers and organic–inorganic hybrid photodetectors [2]. Structural, elastic and electronic properties of Cu based ternary zintl phases KCuX ($\text{X}=\text{Se}, \text{Te}$) have been studied, using first principles methods. It is well known that the standard semi-local GGA underestimates band gaps; therefore, the exchange and correlation effects of self-consistency are also treated by using the modified Becke–Johnson (mBJ) potential [3] by incorporating the relativistic spin orbit coupling. This study reveals that the unexplored KCuX ($\text{X}=\text{Se}, \text{Te}$) compounds are mechanically and dynamically stable and are direct band gap semiconductors. The electron, heavy hole and light hole effective masses were derived from the calculated band structures. The calculated effective mass is directly proportional to the band gap and average nuclear charge of the studied zintl phases. The effective mass results indicate that KCuTe has more dispersive bands than KCuSe which makes the later a better suited material for photovoltaic applications. This work also highlights strain induced tuning of electronic properties which could result in development of these materials in thermoelectric applications.

References

1. J. H. Dughaish, Physica B 322, 205 (2002)
2. B.G. Yalcin, Philosophical Magazine, 96, 2280–2299 (2016)
3. F. Tran and P. Blaha Phys. Rev. Lett. 102, 226401 (2009)

Keywords: Electronic properties, Spin orbit coupling, Effective mass



O2.5

PROSPECTS OF GRAPHENE AND CARBON NANOSTRUCTURES IN THERMAL MANAGEMENT APPLICATIONS

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Graphene, a two dimensional sheet of sp^2 - hybridized carbon with one atom thickness, has become an important material in the technological world owing to its exceptional and unique properties. It has an ultrahigh surface area, highest electrical conductivity, highest Young's Modulus and an excellent thermal conductivity of $3000-5000 \text{ Wm}^{-1}\text{K}^{-1}$. Graphene also shows up nonlinear thermal conductance behaviours like Thermal Rectification (TR) and Negative Differential Thermal Conduction (NDTC) which opens up various possibilities in thermal management applications. Graphene can be used to construct Thermal Rectifiers by physical/ chemical functionalization, introduction of spatial asymmetry in geometry, isotopic defects or by introduction of interfacial structures. In this work various Graphene structures with geometrical asymmetries and interfacial structures are simulated with Comsol Multiphysics Software for their performance as Thermal Rectifiers. They are compared based on Thermal Rectification ratio and various factors which effect its performance was also studied. Based on the simulation results most efficient nanostructures for thermal management applications was proposed.

Keywords: Graphene, Thermal Rectification, Comsol multiphysics

O2.6

MICROSTRUCTURE AND DRY SLIDING WEAR BEHAVIOR OF AUSTEMPERED HIGH SILICON STEEL

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In the present investigation, the influence of austempering temperature and time on the microstructure and dry sliding wear behavior of high silicon steel were studied. The test specimens prepared were initially austenitised at 900 °C for 30 minutes, followed by austempering heat treatment at different temperatures 280 °C, 360 °C and 400 °C respectively for varying austempering durations from 30 to 120 minutes. These samples after austempering heat treatment were subsequently air cooled to room temperature, to generate typical ausferritic microstructures and then to correlate with the wear property. Results show that the specific wear rate increases with increase in both austempering temperature and time. Specific wear rate was found to be

minimum at an austempering temperature of 280 °C, that exhibits lower bainite microstructure with high hardness, on the other hand specific wear rate was found to be high at increased austempering temperatures at 360 °C and 400 °C respectively, due to the upper bainite structure that offered lower hardness to the matrix. The sample austempered at 280 °C for 30 minutes offered superior wear resistance when compared to other austempering temperatures and durations, mainly due to the presence of fine acicular bainitic ferrite along with stabilized retained austenite and some martensite in the microstructure.

Keywords: Austempering; ausferritic; specific wear rate.

O2.7

EFFECTS OF TEMPERATURE AND MULTIAXIAL STATE OF STRESS ON CREEP RUPTURE BEHAVIOUR OF 304HCu AUSTENITIC STAINLESS STEEL

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Increasing efficiency, minimizing CO₂ emission and reduction in coal consumption calls for boiler tube material which can withstand high temperature and pressure, good corrosion resistance and adequate mechanical properties. An advanced Ultra Super Critical (AUSC) power plant designed by the researchers is planned to adopt clean coal technologies by optimizing above conditions. It operates in the steam temperature range of 973-1023K. The critical parts like steam piping and steam turbine requires material of sufficient strength. The 304HCu SS is one of the candidate materials for boiler tubes employed in Advanced Ultra Super Critical power plants. However, boiler tube will suffer multi axial state of stress due to internal pressure, change in cross section, weld joint, presence of notch or hole and microstructural inhomogeneity etc. Notched specimens of different root radius were widely used to simulate multiaxial state of stress in laboratory scale. In the present investigations circumferential-U notches of different root radius (0.25-5mm) were creep tested at both 973 and 1023K along with plain specimens. Material is found to exhibit “Notch strengthening” at both conditions of temperature. The rupture life was found to increase with decrease in notch root radius. However, at 1023K a downward trend was observed after attaining a trend of saturation. Fracture behaviour was studied for different notch root radius at different applied stress by SEM fractograph. Optical and SEM micrograph reported that material is more prone to cavitations and intergranular cracking at 1023K as compared to 973K. Transmission electron microscopy (TEM) was carried out at the notch plane for relatively sharper notches to observe the dislocation substructure study. FE analysis of state of stress has been carried out to understand the variation of different components of stresses across the notch root at both the test temperature. Creep life prediction

under multiaxial state of stress was done by models given by Hayhurst and Cane and compared between two temperature.

Keywords: 304HCu SS, multiaxial creep, Finite element modeling, Life prediction

O3.1

INFLUENCE OF GROOVE ANGLE ON TYPE IV CRACKING BEHAVIOUR OF T91 STEEL WELD JOINT

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Premature failure of ferritic steel welded components in the power plants by Type IV cracking is the major concern. Type IV cracking occurs in the soft intercritical region of heat affected zone (HAZ) in modified 9Cr-1Mo steel due to mechanical strength inhomogeneity across the weld joint. The strength inhomogeneity across the joint produces stress triaxiality during creep, which results in pronounced creep deformation and cavitation in the soft intercritical region of HAZ, leading to the premature type IV failure. Groove angle of the weld joint can alter the degree of stress triaxiality and is expected to influence the type IV cracking behaviour of the joint. In this investigation, creep tests on square butt and V-groove (having face angle of 35°, 45° and 60°) cross weld joint specimens of modified 9Cr-1Mo steel have been carried out at 923 K and 100 MPa stress to assess its effect on type IV cracking behaviour. All the specimens were ruptured by premature type IV cracking by localized deformation in the inter-critical region of the weld joint, at the region which had shown the lowest hardness in the pre-creep condition. The creep rupture life of the weld joints were found to vary significantly with weld groove angle.

O3.2

EFFECT OF CRITICAL CURRENT DENSITY IN THE PHASE DIAGRAMS OF LOW TEMPERATURE SUPERCONDUCTORS, $\text{Ca}_3\text{Rh}_4\text{Sn}_{13}$

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We perform magnetization measurements in different single crystal samples of low temperature type-II superconductors, $\text{Ca}_3\text{Rh}_4\text{Sn}_{13}$. Normally, isothermal magnetization curves of these crystals have two anomalies; second magnetization peak and peak effect. Among the samples, phase diagrams of one particular sets of $\text{Ca}_3\text{Rh}_4\text{Sn}_{13}$ single crystals show positive slopes in their second

magnetization peak curves while other samples show flat second magnetization curves. We observe that the critical current densities of these particular sets of single crystals are different from other samples. The crystal which shows a high critical current density makes a positive slope in its second magnetization peak curve whereas the low critical current density crystal produces a flat second magnetization peak curve. We also examine the underlying reason of different critical current densities of these crystals using X-ray diffraction.

Keywords: Superconductors, Second magnetization peak, Critical current density

O3.3

STRUCTURAL AND ELECTRONIC PROPERTIES OF 1,2-BIS(1H-TETRAZOL-1-YL)ETHANE UNDER HIGH PRESSURE USING DENSITY FUNCTIONAL THEORY

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Recent advances in the field of energetic materials attracted the scientific community by taking leading hands to synthesize materials with high nitrogen content that can lead to higher heat of formation. Especially, Tetrazole are found to be promising Nitrogen rich energetic materials due to their better performance and high thermal stability because of the aromaticity associated with the ring. 1,2-bis(1H-tetrazol-1-yl)ethane (1-DTE)[1] is one among the tetrazole family with 67 w% of nitrogen content in which the $\text{CH}_2\text{-CH}_2$ group connects the two N atoms beside the C atoms on the two tetrazole rings. In the present work, we report the structural and electronic properties of 1-DTE using density functional theory by including weak intermolecular interactions. The

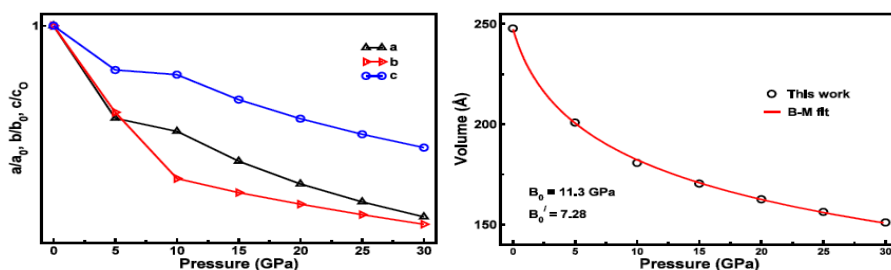


FIGURE 1. Calculated a) normalized cell parameters and b) volume as a function of pressure.

obtained ground state parameters using DFT-D2 method are in good agreement with the experimental data. The pressure dependent lattice constants, compressibility and equation of state are investigated. The bulk modulus (B_0) and its pressure derivative (B'_0) determined by fitting

Birch-Murnaghan third-order equation of state to the volume compression data are found to be 11.3 GPa and 7.28, respectively. The compressibility curves reveal that 1-DTE is highly compressible along crystallographic *b*-axis. It is well known that the electronic band gap obtained from the standard DFT functionals such as LDA and GGA are strongly underestimated, therefore we have calculated electronic properties using semi-local Tran-Blaha modified Becke-Johnson potential. It is found that 1-DTE is an indirect band gap insulator along high symmetric Γ -X direction with a band gap of 4.82 eV.

References

1. T.M. Klapotke and S. M. Sproll, J. Org. Chem, 4284 (2009).
1. B. Yuan and E. R. Bernstein, J Chem Phys, **144**, 234302 (2016)
2. G. Kresse and J. Furthmueller, Phys. Rev. B **54**, 11169 (1996).
3. F. Tran and P. Blaha, Phys. Rev. Lett. **102**, 226401 (2009)

O3.4

SYNTHESIS, MORPHOLOGY AND TOPOGRAPHY ANALYSES OF CERIA-BASED NANOPARTICLES TO BE USED AS LUBRICANT PROPERTY ENHANCERS

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The excessive usage of fossil fuels and crude oil reserves has led to a global need for their conservation. The prime cause of energy loss in a mechanical system is friction and a meaningful solution developed so far is the technique of lubrication. The lubricants added with nanoparticle additives have achieved a predominant position in the field of research and development of sustainable lubricating oils. The efficient physical and chemical properties of metal oxide nanoparticles as lubricant additives have widely extended its purview. However, cost effective synthesis routes and characterization of nanoparticles along with the need for selection of a suitable base-oil is a general issue faced by various researchers. The present work aims to synthesize and characterize ceria-based hybrid nanoparticles for lubricant application. The efficient properties of doped ceria nanoparticles have led to the research on utilization of these types of nanoparticles as lubricant property enhancers. The ceria-based nanoparticles are synthesized through the bottom-up approach of chemical processing namely Precipitation Method (PM). The surface morphology and topography analysis of the hybrid nanoparticles are carried out using High Resolution Transmission Electron Microscopy (HRTEM), Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), Fourier Transform Infrared Spectroscopy (FT-IR), X-Ray Diffraction (XRD) and Zeta

Potential (ZP) analyses techniques. The better control on particle size of PM results in refined and spherically shaped nanoparticles. Further, to improve the dispersion stability of the prepared nanoparticles in the lubricant, a suitable surfactant namely Polysorbate 20 (Tween 20) is used.

Keywords: Nanoparticles, PM, Microscopy, Surfactant.

O4.1

GRAPHENE BASED ELASTOMER WITH Ni AND TiO₂ NANOPARTICLES

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Nanotechnology is an area that has wide range of potential applications. By reducing the size of a particle to nanoscale, its surface area to volume ratio will be increase and more molecules are available to take part in chemical reactions. In this work, reduced graphene oxide (r-GO) is added to natural rubber as fillers. Ni nanoparticles and TiO₂ nanoparticles are added in equal proportion to this nanocomposite to improve its properties mainly shape memory effect. r-GO is added to improve the mechanical strength and the thermal conductivity of the composite. NiTi is a shape memory alloy and thereby by adding Ni nanoparticles and TiO₂ nanoparticles to graphene based elastomer nanocomposite it will show shape memory effect. Properties of the new nanocomposite are compared with the shape memory properties of other alloys like NiTi and FeNiCoTi

O4.2

INVESTIGATION ON THE PROPERTIES OF NATURAL RUBBER/GRAPHENE QUANTUM DOT NANOCOMPOSITE

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Nanomaterials are having the ability to disperse homogenously in the polymeric matrix and share strong binding properties. The chemical physical, electrical, mechanical and thermal properties of the polymers can be enhanced by incorporating nanomaterial as fillers. Polymeric nanocomposites can be prepared by incorporating the filler, graphene quantum dots (GQDs), into the elastomeric

matrix, natural rubber (NR). The reinforcement of GQD into elastomeric matrix leads to change in electrical conductivity, mechanical properties and the resistivity responds to chemicals. This makes the nanocomposite capable of monitoring and sensing toxic as well as non-toxic chemicals and gases in industries and environment, energy and biomedical applications. The structural, morphological, crystalline and electrical properties of the NR/GQD nanocomposite have been studied.

Keywords: Nanocomposite, natural rubber, graphene quantum dots

O4.3

ROLE OF PLANT EXTRACTS IN NANOPARTICLE SYNTHESIS

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The bottom up chemical approaches in the synthesis of nanoparticles has now been widely addressing the environmental issues for depleting the polluting effects and the slogan for the need of alternative routes, the so called ‘eco-friendly approach’ echo from every corners of life. The Alternate techniques replacing the usual chemical methods are called Green synthesis. In this method, the harmful chemical raw materials used in chemical synthesis are completely or partially replaced with bio-reagents such as plant or microorganism extracts. Many a number of studies are being published using plant leaf extracts as one of the raw materials, most probably as the reducing species. Synthesis of zerovalent noble metals and/or metal oxides or metal oxide perovskite structures are possible through green chemistry, wherein the chemical precursor salts are getting reduced under the action of plant leaf extracts. This can be achieved through the simultaneous use of reductants and capping agents and with some chemicals such as sodium citrate, both the functions can be achieved using the same species. The reducing agent provides electrons to the precursor ions. For example, in noble metals it transforms ions in the elemental metal. The capping agent subsequently stabilizes the nanoparticles formed. Thus, the capping and reducing agents can be used together or through one entity and in most cases they are, as the reducing agent transforms the metal ions into elemental metal, which then grows into a particle and the capping agent prevents that particle from growing beyond the nanometric size of interest. The precursor salts in the aqueous solution dissociate into corresponding cationic and anionic radicals. Plant leaf contains high level of phytochemicals, say for example, poly-phenols (Flavonoids). Phenolic compound has hydroxyl and ketonic groups which are able to bind to metals and reduce the metal salt and provide stability against agglomeration. Plant extracts provide protein and enzyme to the aqueous solution of precursor salt in which metal cations combine with the enzyme to form enzyme substrate complex and finally leading to the release of zerovalent metal nanoparticles. The metal nanoparticles combine with the protein released from

the plant extract which subsequently form a protein cap around the nanoparticles. Apart from noble metals, in case of transition metals, there exists a highest possibility to form metal oxides soon after the release of the corresponding zerovalent metal from the enzyme complex. The pH of solution stages a crucial role in such circumstances such that the high pH can cause greater oxidation.

As far as growth is concerned, each particle on nucleation grow on all directions depending up on the synthesis conditions, particularly the temperature of the synthesis employed and the time of synthesis for completion of the reaction. The capping agent or surfactant surrounded by the nucleated particle naturally restricts the particle from growing. Moreover, the steric forces involved in such cases keep the nucleated ligands separated from each other to prevent agglomeration. On the other hand, if one does not use any capping agent/surfactant/stabilizer in the synthesis, still the reaction takes place and particles grow freely. In the process, some particles which are nucleated a little earlier may grab the surrounding particles that nucleated a little later to grow non-uniformly. That is the reason why the particles in the finished product do not look like similar in shape and size in such syntheses processes. Here, what really contributes to agglomeration is that the grown up particles physically attached to each other, become inseparable and look like particle clusters. This may not be suitable particularly for applications like biomedical, cell separation and information storage where the particles should be preferably mono dispersed. In this context, the talk will focus on our attempt to synthesis such nanoparticles using various plant leaf extracts with an ultimate aim to obtain the multiferroic perovskite structures.

O4.4

FLUORESCENCE QUENCHING OF AQUEOUS SOLUTION OF FLUORESCIN DOPED WITH ZnS NANOPARTICLES

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Colloidal semiconductor nanocrystals exhibit excellent optical properties made them useful for optics and optoelectronic applications. In this work energy transfer between Fluorescein dye and ZnS nanoparticles has been investigated using time domain and frequency domain measurements. ZnS nanoparticles were synthesized using hydrothermal method and characterized using TEM and XRD. It was doped in 0.1 M aqueous solution of Fluorescein dye and photoluminescence and life time measurements were made. Emission parameters such as quenching coefficient, energy transfer efficiency were evaluated. The fluorescence quenching and decrease in life time indicate resonant energy transfer between Fluorescein (Donor) and ZnS nanoparticles (acceptor)

Keywords: Energy Transfer, Photoluminescence, Quenching, Life time

O4.5

EFFECT OF FERRITE PHASE ON MAGNETO-ELECTRIC PROPERTIES OF NANOCOMPOSITES OF SODIUM POTASSIUM LITHIUM NIOBATE**R. Rakhikrishna^a, Johny Isaac^b and Jacob Philip^{c*}**^a *Department of Physics, N S S Hindu College, Changanacherry, India*^b *Department of Instrumentation, Cochin University of Science and Technology, Cochin 682 022, India*^c *Amal Jyothi College of Engineering, Kanjirapally, Kottayam 686518, India*

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Multiferroic nanocomposites of Sodium Potassium Lithium Niobate with Cobalt Ferrite or nickel ferrite, with four different molar weight percentages, are prepared by solid state reaction involving co-precipitation and sintering. Structural characterizations of the samples are done using XRD and FT-IR. Magnetic properties of nickel and cobalt ferrite based samples are compared using VSM measurements. The dielectric properties of the samples are measured as functions of frequency, temperature and external magnetic field. After poling, dielectric properties show resonance/relaxation peaks at certain frequencies. The magneto-electric coefficient or the efficiency of the material is measured using a dynamic measurement method. The effect of magnetic hysteresis on magneto-electric behavior of the samples is studied. Values of magneto-electric coefficient obtained for nickel ferrite is larger than cobalt ferrite because cobalt ferrite is magnetically harder than nickel ferrite. These values are comparatively good for the lead free samples prepared by same route. The changes in electrical polarization with the applied magnetic field make these lead free materials promising for the applications like ecofriendly smart sensors and memory devices.

Keywords: Multiferroic materials; Magneto-electric coupling; Sodium Potassium Lithium Niobate; Cobalt Ferrite; Nickel ferrite

O5.1

EXPERIMENTAL INVESTIGATIONS ON A SERPENTINE TUBE TYPE WATER BASED PV THERMAL SYSTEM WITH AND WITHOUT REFLECTORS

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The most inexpensive and effective method to increase the incident solar radiation on the panels is to place reflectors on the sides of the panel so that the diffuse radiation and the radiation falling on the reflectors along its length, at different times of the day can be reflected back to the panels which are made use to produce electricity. Optical reflectors would replace costly PV cell area by cheaper reflector material such as glass mirror, aluminum sheets, stainless steel, acrylic mirror sheets etc. Reflectors can be positioned at an optimum angle to obtain the maximum amount of sunlight. The technique of using this type of reflectors is a lot simpler and less complicated than the existing concentrators and tracking mechanisms. But, while increasing the amount of sunlight onto the panel, the amount of heat that is being produced on the panel also increases. Thus, panel temperature increases simultaneously. So, reflector system should always include a cooling mechanism. Cooling of PV panel not only reduces temperature, but also increases power output and electrical efficiency. This paper discusses about the study conducted on cooling of PV panel with and without planar reflectors.

O5.2

STUDY ON TENSILE CHARACTERISTICS OF CARBON-KEVLAR HYBRID COMPOSITE AND KEVLAR EPOXY COMPOSITES

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Composites have been widely used in many industries due to their exceptional properties that even replace steels and other materials. Due to their high strength to weight ratio and other characteristics has made them to be used defence and aerospace industries. The low cost and easy fabrication process is also a factor for their extensive use. Currently hybridization of composites has become an area of wide research to find out suitable combinations to give

specific properties. The study focuses on hybridization of Carbon and Kevlar and Kevlar epoxy composites which is widely used in both defence and aerospace industries.

Vacuum bagging process is an efficient method which is widely used in aerospace industries for fabrication of different parts. The process uses vacuum as a clamping mechanism by creating a vacuum chamber which presses the composite till curing is done. Thus the specimens for tensile test were prepared using vacuum bagging process. The material was then cut for the test to a dimension according to ASTM D3039 specification the dimension of the specimen is 250mm x 250mm x 3mm, which is a standard followed for tensile test for polymer composites. The test was conducted on UTM. Three specimens of each hybrid and Kevlar epoxy composite were tested. The result showed that the hybrid composite was able to withstand large amount which is approximately 4190N which produced an elongation of 5.9% and Kevlar epoxy composite withstood a load of 3300N which caused an elongation of 27.9%. It was also noted that hybrid composite has ultimate stress more than 27% than Kevlar epoxy composite. Numerical simulation of the tensile test was done in ABAQUS Cae 6.14. Shell element was used for modelling the composite and total number of elements was 410 with number of nodes 499. Carbon layup was in 0° and 90° were as for Kevlar it was 0°, 45°, -45°, 90°. The results from numerical analysis and test data was compared and from the test maximum stress for hybrid was found to be 79.5MPa and from analysis 91.6MPa. For Kevlar epoxy composite it was 56.3MPa from the test and 60.1MPa from the analysis.

Keywords: Carbon and Kevlar composites, Vacuum bagging, tensile test

O5.3

AN ENHANCEMENT IN CREEP STRENGTH OF MODIFIED 9Cr-1Mo STEEL WELD JOINT

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Modified 9Cr-1Mo steel (T91) derives its strength from tempered martensitic lath structure having transformation induced high dislocation density, $M_{23}C_6$ precipitate in the grain and sub-grain boundaries, MX precipitate in the intra-lath regions predominantly, which were obtained generally through normalizing and tempering (NT) treatment. Modification of microstructural constituents in the steel during weld thermal cycles resulted in generation of soft zone in the heat affected zone of the joint close to base steel by coarsening of precipitates and subgrain formation with reduced dislocation density. These results in mechanical properties trough in the intercritical region of the HAZ, which led to premature type IV failure of the weld joint under creep. In order to improve the type IV cracking resistance of the steel weld joint, the thermo-mechanical treatment (TMT)

has been carried out on the steel to enhance the MX precipitation. Weld joint of NT and TMT steels have been fabricated using EB welding. Significant variations of microstructural constituents and hardness across the joint, soft zone formation in the ICR have been observed in both the joints. Creep test have been carried out on NT and TMT steels joint at 923K and 110 - 100 MPa applied stress. Creep rupture life of the TMT weld joint was significantly higher than the NT steel weld joint. The enhanced MX precipitation through TMT processing and reduction in coarsening of $M_{23}C_6$ precipitate under thermal cycle resulted in improved creep rupture life of TMT joint than NT weld joint.

O5.4

THERMAL CONDUCTIVITY OF SELECTED NANOFLUIDS EMPLOYING TRANSIENT HOT WIRE TECHNIQUE

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Thermal conductivities of gold, silver and ZnO nanofluids, prepared by dispersing nanoparticles of the respective materials at different volume fractions in the base fluid (water) were determined experimentally and calculated theoretically. The experimental values were obtained from an apparatus that was designed and fabricated for this purpose, following the transient hot wire technique, and the theoretical values were obtained following three theoretical models developed to evaluate effective thermal conductivity of mixtures. The three theoretical models used were Maxwell-Garnett model, Hamilton-Crosser model and Bruggeman model, and the agreement of the theoretical values provided by these models with experimentally obtained values have been analysed and presented.

O6.1

SOLVENT SENSING CHARACTERISTICS OF IONIC LIQUID MODIFIED MWCNT BASED SBR NANOCOMPOSITES

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Polymer nanocomposites play a significant role in the science and technology of present nanocomposite research due to its multi-functional behaviour and potential applications in various fields. Realisation of a well dispersed SBR based polymer nanocomposite has been limited because of issues of uniform dispersion of fillers in the rubber and the sufficient interfacial compatibility between the filler and the polymer. Here special emphasis has been

given to surface modification of MWCNT by ionic liquid, a green approach among various functionalization methods. The synergic effects between ionic liquid and MWCNT improved mechanical, electrical and surface characteristics of nanocomposites. The high electrical conductivity of fabricated nanocomposites pioneers a new platform for development of high performance materials for solvent sensing application and has never been addressed. The solvent sensitivity of the composite samples was noted from the sudden variation in electrical conductivity which was due to the breakdown of the filler networks during swelling in different solvents.

O6.2

STUDY OF BIAS DEPENDENCE OF TUNNELING MAGNETORESISTANCE IN Co/MgO/Co MAGNETIC TUNNEL JUNCTIONS USING FIRST PRINCIPLES CALCULATIONS

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This paper reports the bias dependence of tunneling magnetoresistance in Co/MgO/Co magnetic tunnel junctions (MTJs) using first principles SGGA band structure calculations at four different temperatures. The Co/MgO/Co tunnel junction has been simulated at four different temperatures to obtain the I-V and dI/dV -V characteristics with parallel and anti-parallel magnetization states, respectively. The TMR ratios have been computed at all four different temperatures. It is seen that temperature doesn't seem to greatly fluctuate the TMR ratios of this magnetic tunnel junction, thereby making it suitable for applications over a wide range of temperatures. For the same four temperatures, the tunnel junction has been simulated for increasing insulator thicknesses. The exponential increase in resistance in both parallel and antiparallel magnetization states has been observed with an increase in the insulating layer thickness. The effect of increasing insulator thicknesses on the TMR ratios at all the four temperatures has also been presented in this paper. The study of bias dependence of tunneling magnetoresistance presented in this paper aptly justifies the application of Co/MgO/Co MTJs in Magnetoresistive Random Access Memories.

Keywords: Magnetic Tunnel Junctions; SGGA; bandstructure; TMR; Co/MgO/Co; Magnetization

O6.3

GREEN SYNTHESIS OF MAGNETIC IRON NANOPARTICLES AND ITS ENCAPSULATION FOR WATER TREATMENT

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Iron nanoparticles of its physiochemical properties made which in the applications of catalysis, drug delivery, environmental remediation and water treatment so on. Iron nanoparticles are most commonly synthesized by chemical precipitation method. Here an iron precursor is reduced by using reducing agents but its environment toxicity and cost limit its application. . Now a day's the green route synthesis of iron nanoparticles which are economical and environment friendly. In this study, the leaf extract of papaya leaves is used for the green synthesis of magnetic iron nanoparticles by a simple, economic and environmental friendly way. The prepared nanoparticles are encapsulated by using alginate solution and are used for the adsorption study. The Response Surface Methodology (RSM) is widely using optimization technique applied and the optimization parameters are determined for water treatment.

Keywords: Green synthesis, Adsorption, RSM

O6.4

EFFECT OF PROCESS PARAMETERS ON THE AGEING PROPERTIES OF Sc INOCULATED CAST Al-Zn-Mg ALLOY

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Al-Zn-Mg alloys of 7xxx series are used in aerospace engineering due to their high-strength-to-weight ratio and good fracture toughness. Al-Zn-Mg alloy is exhibited strong age-hardening properties due to the Sc (0.39 wt%) inoculation effect which is due to the decomposition of the supersaturated solid solution (SSS) and the formation of a fine distribution of coherent GP (Guinier-Preston) zones precipitates, semi coherent η precipitates (metastable) and Al_3Sc ($L1_2$) precipitates. The influence of various process parameters on the microstructure and tensile properties of the cast Al-Zn-Mg alloy are studied by TEM, FESEM, DSC, and Vicker's hardness measurements. In addition, the ageing sequence consists of three steps such as solutionizing ($465^\circ C/1h$) then immediate water quenching (T_4), natural ageing for 3 days at room temperature, and artificial ageing at $140^\circ C$ for 6h. The microstructure at peak strength is shown to depend on the mainly dissolution of GP zones, nucleation of η and Al_3Sc precipitates or formation of GP zones, nucleation of dislocations and dislocation with Al_3Sc particles interaction. GP zones are

formed at room temperature ageing, and become unstable at above about 100°C which is usually well-known as effect of reversion for Al-Zn-Mg alloys. At higher temperature around 140°C the η transition phase is being formed and thermal stability of Al_3Sc phase at above 300°C. The aim of this paper is to investigate in detail the ageing behaviour of cast Al-Zn-Mg alloy and to understand the age-hardening mechanism at 140°C ageing condition.

Keywords: η precipitates, Al_3Sc particles, Vicker's hardness, artificial ageing at 140°C.

P1

SYNTHESIS OF PURE AND SILVER DOPED ZINC OXIDE NANOPARTICLES USING CO-PRECIIPITATION METHOD AND ITS CHARACTERIZATION

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Pure and silver doped Zinc oxide nanoparticles were successfully synthesized by co-precipitation method from zinc sulphate, sodium hydroxide and silver nitrate as precursors. PEG was used as a chelating agent. The synthesized samples were characterized using X-Ray Diffraction, Fourier Transform Infra Red, Transmission Electron Microscopy and Photoluminescence. The X-Ray analysis shows that all the diffraction peaks of ZnO matched well with the JCPDS data. The sample Ag doped ZnO also reveals hexagonal wurtzite structure of ZnO. From the XRD data, the average crystallite sizes of ZnO were found to be 24 nm. TEM images reveal that the synthesized particles are nearly rod like structure with breadth 24 nm and length in the micrometre range. The crystallite size calculated using the Debye Scherrer's equation and the TEM data matches very well. ZnO vibrational modes are more prominently observed in the FTIR spectrum. Ag doped ZnO showed a significant modification in the emission spectrum of ZnO. Nano-structured pure ZnO powders showed luminescence in the UV and visible regions which can be used for the fabrication of new generation UV sources.

Keywords: ZnO, nanoparticles, co-precipitation

P2

SYNTHESIS AND CHARACTERIZATION OF Pt-Fe₂O₃ NANOPARTICLES AND ANTIBACTERIAL ACTIVITY

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Nanocrystalline Pt-Fe₂O₃ was effectively synthesized by sol-gel method via citrate sulphate precursors. The prepared products further characterized by powder X-ray diffraction (PXRD), UV-Visible diffuse reflectance spectroscopy (DRS) and Scanning electron microscope (SEM), Fourier transformer Infrared spectroscopy (FTIR). X-ray diffraction pattern confirmed the formation of single phase Pt-Fe₂O₃ nanoparticles. FESEM images indicates the obtained samples are micro porous sphere like morphology and its grain size will be in the range of 80-200nm. An

optical property of Pt-Fe₂O₃ shows an energy band gap as 3.20eV. The investigated antibacterial studies confirmed that the particles are well suitable for anticancer agent.

Keywords: Iron oxide, semiconductor, sol-gel method, optical property.

P3

EFFECTS OF T6 HEAT TREATMENT AND STRAIN RATE ON THE TENSILE PROPERTIES OF TIG WELDED AL-6063 ALLOY JOINTS

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The paper was aimed at investigating the effect of various strain rates on the tensile properties of the TIG welded 6063 alloys. The alloy samples were tested at two conditions, as-welded and heat treated, for different strain rates of 0.5, 1.0, 2.0, and 10 mm/min. The heat treatment parameters for the welded alloy samples were selected based on various experiments involving different solutionizing and ageing temperatures and times. The results indicate that the tensile strength of the non-heat treated welds behaved variedly at different strain rates. The tensile strength of non heat-treated weld sample tested at 0.5 mm/ min was 58 MPa and increased to 68 MPa on heat treatment. The heat treated alloy welds showed a constant increase in the tensile strength and elongation with increase in strain rate. The improvement in weld strength with heat treatment was due to the homogenous and fine precipitation of the precipitates in the weld.

Keywords: Tensile strength, heat treatment, TIG welding, aluminum alloys

P4

BIOSYNTHESIS OF SILVER NANOPARTICLES USING *NIGELLA SATIVA* SEED EXTRACT AND EVALUATION OF ITS ANTIOXIDANT AS WELL AS PHOTO-CATALYTIC ACTIVITY

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Biosynthesis of silver nanoparticles using aqueous extract of *Nigella Sativa* seed under sunlight and heating was analysed in this study. Irradiation of sunlight shows better formation of silver

nanoparticles. The different parameters were optimized for the synthesis of silver nanoparticles like the concentration of *Nigella Sativa* seed extract, concentration of silver nitrate solution, incubation time and reaction temperature. Green synthesised nanoparticles can be used effectively for the biological use. The antioxidant activity of the nanoparticles was evaluated using the 2, 2-Diphenyl-1-picrylhydrazyl (DPPH) radical. The photo degradation of a dye – coomassie brilliant blue G-250 using the biosynthesised Ag nanoparticle was also evaluated. The DPPH assay and the photo-degradation was analysed using UV-Visible spectroscopy. The biosynthesised nanoparticles were characterised using UV-Vis spectrophotometry, FTIR spectrophotometry, XRD. The size of the particles was analysed by SEM and TEM. The results shows that the *Nigella Sativa* seed extract can be effectively used for the synthesis of silver nanoparticle and the green synthesised Ag nanoparticles can be used as an anti-oxidant as well as a photo-catalyst.

Keywords: Nigella sativa, Silver nanoparticles, anti-oxidant

P5

GREEN SYNTHESIS OF SILVER NANOPARTICLES USING CINNAMOMUM TAMALA LEAF EXTRACT AND EVALUATION OF ITS ANTIOXIDANT ACTIVITY

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The field of nanotechnology is the most active area of research in modern materials science. Nanoparticles rapidly gaining importance in various fields such as electronics, catalysis, chemistry, energy and medicine. Among several noble metal nanoparticles, silver nanoparticles have attained a special focus due to its unique properties such as chemical stability, good conductivity, catalytic activity, antibacterial, anti-viral, antifungal and anti-inflammatory activities. Conventional methods of synthesis of silver nanoparticles involve use of toxic chemicals which is non-ecofriendly. Therefore, in the present study designed a cost effective and environment-friendly technique for green synthesis of silver nanoparticles from silver nitrate (AgNO_3) solution using *Cinnamomum tamala* leaf extract and to evaluate the antioxidant activity in vitro. Various physicochemical parameters are evaluated and optimized for the design of novel green synthesized silver nanoparticles including the concentration of *Cinnamomum tamala* extract, concentration of silver nitrate solution, incubation time and reaction temperature etc. The synthesized nanoparticles were characterized using UV-Vis spectrophotometry, FTIR spectrophotometry XRD and SEM. The antioxidant activity of synthesized silver nanoparticles was investigated by 2, 2-Diphenyl-1-picrylhydrazyl (DPPH) assay.

Keywords: Cinnamomum Tamala, Silver nanoparticles, anti-oxidant activity

P6

**COMPUTATIONAL STUDY ON MECHANISM OF HYDROXYL RADICAL
SCAVENGING BY MELATONIN AND N-ACETYL TRYPTOPHAN**Aiswarya Purushothaman, Achutha. A. S, Deepa Janardanan*Department of Chemistry, School of Physical Sciences, Central University of Kerala*

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The hydroxyl radical scavenging activities of two tryptophan derivatives- melatonin and N-acetyl tryptophan- have been investigated using density functional theory. The mechanism involves 4 steps: initial radical addition to position-3 of the indole ring, tautomerization, ring formation and finally, addition of a second .OH radical, leading to a cyclic end product. Of these the initial step is found to be barrier-free. The tautomerization step has the highest barrier energy and can be considered as the rate determining step for both the indoleamines. The final addition of second .OH radical to form cyclic 3-hydroxy melatonin and cyclic 3-hydroxy-N-acetyl tryptophan with the elimination of a molecule of water is found to be barrier-less. Solvent effects of the aqueous medium on certain reaction barriers are appreciable. Comparative simulations on the interaction of hydroxyl radical with melatonin and N-acetyl-tryptophan reveal that melatonin has lower energy pathway compared to Nacetyl tryptophan. If both the melatonin and N-acetyl tryptophan metabolites formed ultimately can be found to be non-toxic, these can be used as medicatives against oxidative stress.

Keywords: Melatonin, N-acetyl tryptophan, hydroxyl radical scavenging activity.

P7

**COMPUTATIONAL STUDY ON FATE OF THE CRIEGEE INTERMEDIATES
IN THE ATMOSPHERE**Shashikala K, Sruthi T P, Deepa Janardanan*Department of Chemistry, School of Physical Sciences, Central University of Kerala*

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The generation and decomposition of Criegee Intermediates (CIs) from propene (A) and 2- methyl propene (B) with ozone have been investigated using density functional theory. Unimolecular decomposition of Criegee intermediates and its reactions with species like H₂O may significantly alter tropospheric chemistry through the formation of organic acids and OH radicals. A total of four types of reaction pathways were modelled, where the first step involves the formation of Criegee Intermediates (CI). Three different CIs were formed from the two alkenes: Acetyl(CI1), Formyl(CI2), and Dimethyl(CI3). The further reactivity of these intermediates was investigated as three pathways (a) Unimolecular Decomposition, (b) Water Assisted Decomposition, and (c) Generation of OH radicals. We found that unimolecular decomposition pathway (a) as well as OH

radical generation pathway (c) proceeds with significantly high barriers in comparison to the bimolecular decomposition pathway (b) assisted by water. While pathways (a) and (c) have over all barriers of 20-30 kcal/mol, pathway (c) has very lower barriers (4-9 kcal/mol) and is the most favoured on energy grounds. Thus, our study demonstrates the influence of water in driving the reaction to new pathways that are otherwise not available. Water also assists the reaction by reducing the activation barriers significantly. Thus we can conclude that, once water is present in the vicinity of CIs formed from alkenes and ozone, it will definitely drive the mechanism through the lower energetic bimolecular pathway and would result in the formation of acid products.

Keywords: Criegee intermediates, decomposition pathway.

P8

GRAPHENE-Mn₃O₄ NANOCOMPOSITE AS EFFICIENT ANODE MATERIAL FOR LITHIUM ION BATTERY

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With the global increase in energy demand, there has been tremendous focus on developing advanced electrode materials for rechargeable Lithium ion batteries. Nanostructured metal oxides have been studied with great interest as anodes for lithium ion battery, owing to their high theoretical specific capacities.¹ Among various transition metal oxides, Mn₃O₄ is worth investigating because of its high theoretical capacity, low toxicity, low cost and increased abundance.² However the poor conductance and capacity fading with cycling still remain a major challenge. Graphene/ metal oxides nanocomposites have been recently explored as efficient electrodes for Li-ion battery and have been shown to improve the device performance.³ Here we report the synthesis of Mn₃O₄ nanostructures with a novel morphology comprising of nano octahedrons embedded in nanorods *via* hydrothermal method. Further, Graphene- Mn₃O₄ nanocomposites have been prepared and their electrochemical characteristics as Li-ion battery anodes are studied. The structural and morphological characterization have been performed by using X- Ray Diffraction (XRD), Field Emission Scanning Electron Microscopy (FESEM), High Resolution Transmission Electron Microscopy (HRTEM), Infra-Red (IR) spectroscopy, Raman spectroscopy and Brunauer–Emmett–Teller (BET) surface area. Graphene-Mn₃O₄ nanocomposite electrode showed excellent electrochemical performance with a good cycling stability and rate performance. The interaction between reduced graphene oxide and Mn₃O₄ nanostructures results

in synergistic effects of improved reaction kinetics owing to better electrode/electrolyte interface and improved electronic/ionic transport.

References

4. A.L.M. Reddy, S. Gowda, M.M. Shaijumon and P.M. Ajayan, *Adv. Mater.* 24 (2012), 5045-5064
5. K. Zhang, X. Han, Z. Hu, X. Zhang, Z. Tao, J. Chen, *Chem Soc Rev*, 44 (2015) 699-728.
6. H. Wang, L.-F. Cui, Y. Yang, H. Sanchez Casalongue, J.T. Robinson, Y. Liang, Y. Cui, H. Dai, *J. Am. Chem. Soc.*, 132 (2010) 13978-13980.

P9

VISCOSITY, DIELECTRIC PERMITIVITY AND ELECTRICAL CONDUCTANCE MEASUREMENTS OF IONIC LIQUID BASED IRON OXIDE MAGNETIC NANOFLUIDS

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An evaluation of viscosity, dielectric permittivity and electrical conductance of iron oxide magnetic nanofluids (MNFs) synthesized using 1-Butylpyridinium bromide (bpyBr) ionic liquid (IL) via one step microwave irradiation was carried out in this work. Viscosity curves of these materials were measured in shear rate range from 1 to 1000 s⁻¹ at constant temperature of 35°C (308.15 K). The dependence of viscosity on temperature was also examined in temperature range from 35°C (308.15 K) to 70° C (343.15 K) with 1 K per minute step. Samples exhibit Newtonian nature, but studies have shown unexpected rheological behavior of material. Viscosity decreases with fraction of nanoparticles in nanofluids. Electrical properties were measured by two parallel plate method. All measurements were performed at controlled temperature and frequency of electric field. The temperature was varied in the range from 0°C (273.15 K) to 100°C (373.15 K) with 5 K step. The frequency was changed from 0.1 Hz to 10 MHz, in 73 steps. Studies have shown a strong correlation between electrical properties, temperature and frequency, especially in low-range frequency of electric field.