Abstract ID: 100

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Thin Films and Nanomagnets

Keywords: Zinc chromite, Spinel, Thin film, MOCVD, Single Solid Source Precursor, RBS

Synthesis and Characterization of Zinc Chromite Nano-structured Spinel Thin Film Prepared by MOCVD via a Single Solid Source Precursor

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The use of multi-source precursor for thin film deposition can lead to non-uniformity in morphology, presence of unwanted phases in the structure, lack of reproducibility in composition, among others. In this study, the deposition of zinc chromite thin film from single solid source precursor, through metal organic chemical vapor deposition (MOCVD) on sodalime glass substrate, at deposition temperature of 420 oC was reported. The single solid source precursor, zinc chromite acetylacetonate was prepared from commercially available reagents. The film was characterized using Rutherford backscattering spectroscopy (RBS), X-ray diffractometry (XRD), scanning electron microscopy (SEM), UV-visible spectroscopy and four-point probe technique. RBS analysis gave a well-defined stoichiometry of ZnO.Cr2O3 with a thickness of 140 nm. The XRD pattern confirmed the nano-crystalline nature of the film with the formation of a cubic phase with a space group Fd-3m of the spinel ZnO.Cr2O3 structure. SEM micrograph revealed a network of overlapping nano-sheets, which are homogeneous, crack-free, uniformly distributed and contained no voids. Optical characterization revealed a transmittance of about 80% while the absorption spectrum exhibited a sharp absorption edge around 420 nm. A direct band gap of 2.95 eV, Urbach energy of 0.08 eV and steepness parameter of 0.3125 were also obtained from the analysis of the optical data. Electrical characterization showed that the conductivity value is of the order of 10-2 (Ωm)-1 across the temperature, in which electrical conductivity occurred by thermal activated polaron hopping with activation energy, Ea of 0.24 eV.

Abstract ID: 101

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: non-locality-in-time; nanoscale; Landau levels

NONLOCALITY AT NANOSCALES SYSTEMS

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Nonlocality is the most fascinating and poorly understood phenomenon in quantum theory, and it generally manifests when measurements (in space or in time) are obtained based on two or more isolated quantum mechanical systems. We discuss the implication of a nonlocal-in-time uncertainty relation at low-dimensional and nano scales. We compute quantum corrections to Landau levels and we constrain our results with the scanning tunneling microscope experiment.

Abstract ID: 102

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: Photo-electrochemistry, Catalysis, Hydrogen fuel

From Photo-electrochemical Water Splitting to Strategies for Co-Catalyst Design

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The oxygen evolution reaction in photo-electrochemical water splitting is a complex four-electron process that requires multiple surface intermediates that facilitate interfacial charge transfer with the reactants from the electrolyte. On the other hand, those intermediates can also serve as recombination centers for photo-generated charge carriers, which result in large overpotential and efficiency losses. H2O2 is a sacrificial reductant that is often used as a hole scavenger to gain insight into photoanode properties and specifically into recombination. In this talk, I will focus on a distinct mechanism of H2O2 photo-oxidation on haematite (α-Fe2O3) photoanodes and its relation to co-catalysis. Based on photocurrent voltammograms that display non-monotonous behavior upon varying the H2O2 concentration, we postulate a nonlinear kinetic mechanism involving two reaction sites as in Langmuir–Hinshelwood reactions. The devised kinetic model reproduces our main observations and predicts the coexistence of two surface reaction paths (bi-stability) in a certain range of potentials and H2O2 concentrations. Not only that this prediction is confirmed experimentally by observing a hysteresis loop in the photocurrent voltammogram but also it opens new vistas to understand charge transport at the interface. In the end, I'll show why the current work provides a plausible insight into the integration of co-catalysts via concerted interactions, similarly to the two-site H2O2 photo-oxidation reaction.

Abstract ID: 103

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Liquid electrolytes, ionic liquids, polymer electrolytes

Keywords: Electrolytes, Ionic liquids, Porous electrodes, Energy Storage

From Solvent Free to Dilute Electrolytes and Template Free Formation of Mesoporous Structures for Energy Storage

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Concentrated electrolytes are being examined for a broad range of applications and specifically for energy-related devices, examples of which include dye-sensitized solar cells, fuel cells, batteries, and supercapacitors. Optimizing the design of these devices requires a mechanistic understanding of the spatial ionic arrangement and charge transport. Although the physicochemical aspects of electrolyte solutions have been extensively studied, recent experimental and computational results expose knowledge gaps in the underlying basic science.

I will present a novel self-consistent spatiotemporal framework for a ternary composition that comprises ions and solvent employing free energy that consists of short- and long-range interactions, along with an energy dissipation mechanism obtained by Onsager's relations [1]. The model equations are designed to pave the road toward a realistic description of concentrated electrolytes and electrochemical applications thereof, by addressing: (i) explicit densities of electrically positive, negative, and neutral subsets (aqueous or organic carriers), (ii) finite-size (steric) effects, (iii) selective energy dissipation to reflect mass transport, and (iv) macroscopic self-assembly. At low concentrations, the theory naturally relaxes to the classical Poisson-Nernst-Planck equations. In the end it will be shown how the above has led to phase separation at the electrode-electrolyte interface (EEI) that is accompanied by deposition of porous structures of micrometer size on the electrode. The finding of an electrochemically induced phase separation not only brings a paradigm shift in understanding the EEI in ionic liquids but also provides alternative strategies toward designing porous surfaces [2]

Abstract ID: 104
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Polymeric composites
Keywords: Polytriazins, Plastics, Combustion Fuels, Energy Storage

Functional materials for smart plastics, and beyond: Morpholino-poly(piperazinyl-morpholinyl-triazins)

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Plastics, the polymer composites, perhaps the smartest materials ever created in recent times have enabled quantum leaps possible in our evolution and life-style, in shortest possible period of history; their worst curse being that they are too good to be true. However, there are some major issues with plastics such as a) visible and invisible degradation, of both polymer and the ingredients, in inevitable melt-processing, (largely underestimated), b) potential fire hazard while-in-use, being basically solid fuels and c) ultimate disposal of, after-the-use, as waste (not being properly addressed)1-3.

MCA technologies GmbH in Switzerland has developed an environmentally friendly technology that on one hand provides safety in processing and imparts a sustainable fire-safety-in-use to plastics, and on the other hand, it enables their ultimate environmentally friendly disposal as waste, coupled with simultaneous generation of usable energy4.5. The knowledge & experience thus gained from energy extraction of waste plastics could provide guidelines to increase the efficiency of energy production and reduction of emissions from combustion fuels in general. The technology is also intended to safeguard against open burning of plastic waste that can lead to flashover and forest fires.

The chemistry and the working mechanism principles of the technology, applicable as well to alleviate the fire-hazard of lithium ion batteries, will be presented at the symposium.

Key Words: Polytriazins, Plastic Processing, Safety-in-use, Waste Disposal. Combustion Fuels, Energy Storage

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Abstract ID: 105

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Mechanical and Thermal properties of graphene, Mxenes and other two-dimensional materials

Keywords: Nanostructure, Heat Capacity, Bulk Modulus, Thermal Conductivity

Theoretical Computation of Mechanical and Thermal Properties of Copper Nanostructures using Density Function Theory

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On the basis of density functional theory, structural, mechanical, thermal, electronic, and transport properties of Cu nanowires (NWs) with different geometry have been analyzed. The band structures of different geometry confirm that all nanowires are excellent conductors in nature. The electronic thermal conductivities of Cu nanowires have low value than that of the bulk form of Cu. Heat capacity also found low in comparison to bulk and increased with temperature, whereas the Seebeck coefficient enhances and increases with temperature. The obtained energy volume relations using third-order Birch-Murnaghan Equation of State (EOS) have been fitted and find the bulk modulus and its first pressure derivatives at zero pressure. The compression behavior and pressure-dependent bulk modulus of all the nanostructures with the help of Birch-Murnaghan EOS are computed. Our results signify that Cu nanowires have potential application in electronics devices and nanoelectromechanical structures.

Abstract ID: 106

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Graphene, heterostructures, flexible electronics, biomedical applications, inkjet printing

Water-based and biocompatible 2D Inks: from Fully Inkjet Printed Heterostructures to Biomedical Applications

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Solution processing of graphene [1] allows simple and low-cost techniques such as inkjet printing [2, 3] to be used for fabrication of heterostructures of arbitrary complexity. However, the success of this technology is determined by the nature and quality of the inks used.

In this work we show a general formulation engineering approach to achieve highly concentrated, and inkjet printable water-based 2D crystal formulations, which also provide optimal film formation for heterostructure fabrication [4]. Examples of all-inkjet printed devices, such as large area arrays of photosensors on plastic [4], programmable logic memory devices [4], strain sensors on paper [5], capacitors [6] and transistors [7] will be discussed.

In addition, our approach allows easy production of defects-free and biocompatible graphene flakes with positive or negative charge [4,8-10], which can be used to elucidate the effect of surface charge on cellular internalisation and other biological interactions.

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Abstract ID: 107

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Zinc Oxide Thin film, Doping, Absorbance, Reflectance, Transmittance, Transmittance and Band-gap

THE OPTICAL CHARACTERISTICS OF ZnO THIN FILM DOPED WITH ALUMINUM

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In this work, ZnO thin film doped with Aluminium was studied. ZnO was doped with percentage of Al doped given as (0.1, 0.2 and 0.3M) respectively. The thin films were deposited on a glass substrate using Chemical bath deposition technique. The solutions were prepared using zinc sulphate, ammonia provided oxygen ion while Hexamine was used as the ligand and aluminium nitrate was used to provide during doping Al ions. The optical characteristics were investigated using UV-VIS spectroscopy in which the films were seen to have low absorbance, reflectance and relatively high transmittance within near ultraviolet to near infra red region. The result also shows that the energy band gap was direct with values in the range of 3.5ev to 3.9ev and very high optical conductivity.

Abstract ID: 108

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Non-destructive Inspection Techniques for Composite Materials and Structures

Keywords: neutron Compton scattering, neutron diffraction, ab initio lattice dynamics, proton conductors

A mass-selective view of local binding and nuclear dynamics in a BaZr0.7Ce0.2Y0.1O3-o proton conductor as observed by neutron diffraction

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The unique combination of techniques consisting of neutron Compton scattering and neutron diffraction [1-4] have been employed to study a novel proton-conducting system, the hydrated BaZr0.7Ce0.2Y0.103-o (BZCY72), at temperatures between 70 K and 300 K. Neutron data analysis, augmented with density functional theory modelling of lattice dynamics, has enabled a mass-selective view of the combined thermal and nuclear quantum effect on local effective binding. An increased anharmonic character of the lattice dynamics and local binding of the framework atoms is revealed above the orthorhombic to rhombohedral phase transition at 85 K, whereby a subtle interplay between mode hardening and softening with increased temperature tunes the effective local binding of nuclear species. The anharmonic effects seem to be most pronounced in the case of oxygen and cerium. Our analysis strongly suggests the existence of a single type of trapped protons and trap proton sites in the room-temperature non-conducting phase of BZCY72. The protons at room temperature possess insufficiently high kinetic energy to overcome the local barrier for long-range diffusion but enough to perform transfer between different trap sites. Ionic conduction in BZCY72 would then most likely involve two distinct proton types, the ones trapped around the edges of Y06 octahedra, and the remainder formed of protons located near the Zr06 and Ce06 octahedral edges, the sites that would favour mobile protons. The apparent proton conductivity would then result from a subtle interplay between the population size and mobility of the trapped and free proton fraction as a function of temperature.

Key Words: neutron Compton scattering, neutron diffraction, ab initio lattice dynamics, proton conductors

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Abstract ID: 109

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Materials for Memory and Computation

Keywords: Bio-organic Material, Artificial Synapse, Resistive Switching, Metal-Insulator-Metal

Effects of Drying Time on Acemannan-Based Artificial Synaptic Behaviour for Neuromorphic Computing Application

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Neuromorphic systems that emulate human brain functionalities by enabling massive neural-network parallelism are regarded as promising systems that can overcome the limitations of conventional digital computation. The construction of artificial synaptic devices that exhibit memory and learning functions, mimicking biological synapses, is a vital step for the realization of bioinspired neuromorphic systems. Bio-organic materials, as sustainable and biodegradable materials, are gaining preferences as alternatives to inorganic materials for the fabrication of artificial synapses. Extracts from natural Aloe-Vera and subsequently transforming into functional thin-film has proven to be a potential replacement as either active or passive layer in electronic devices. There are two major polysaccharides that play a major role in the dielectric properties of Aloe-Vera, namely Acemannan and Pectin. Here we propose an artificial synaptic device based on Acemannan monomer (D-mannose) that have been dried at different duration (3 to 8 hours). D-mannose is an abundant organic polymers on Earth and is biodegradable, biocompatible, in addition to being environmentally friendly. The as-proposed device, dried at an optimum time of 7 hours, exhibits essential synaptic behaviours, such as, short-term plasticity (STP), long-term plasticity (LTP), STP-to-LTP transition, paired-pulse facilitation (PPF) and post-tetanic potentiation (PTP). The results from the electrical measurement confirm the viability of using D-mannose as an active layer in the fabrication of artificial synaptic devices for neuromorphic systems.

Abstract ID: 110
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Porous and cellular materials
Keywords: Geopolymerization, Foaming, Inorganic, Lightweight

Investigation of cellular building materials using image processing techniques

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This paper investigates the development of cellular foam boards, using perlite wastes as raw material. This type of lightweight materials combines the geopolymerization technology with the foaming process. The mechanism of foaming is based on the generation of a gas that is retained by the geopolymer matrix in the form of individual or interconnected voids. In this study, the inorganic foaming agent is hydrogen peroxide (H2O2), which is added into the initial paste in different quantities by mechanical stirring. The produced porous materials have effective densities between408–476.5kg/m3, thermal conductivities between 0.076–0.095W/m.K and different type of microstructure, depending on the concentration of the activator and the foaming agent content. To assess the porosity and the size distribution of the voids, image processing techniques were applied on digital images of the samples. According to these results, the synthesized lightweight materials exhibit similar or even better thermal properties than the current concrete porous materials.

Abstract ID: 111

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Industrial applications of composite materials

Keywords: 4-aminoantipyrine; Adsorption; Pharmaceutical waste; Vermiculite; Wastewater

Chemically modified vermiculite clay: A means to removing emerging contaminant from polluted water system in Africa and a key to water policy advocacy

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Unreliable water treatment technique and lack of guidelines/policy have been identified as major hindrances to clean drinking water in most African countries like Nigeria. The presence of organic compounds in the environment is of increasing concern due to their eco-toxicological effects. Some of these organic compounds are pharmaceutical agents with therapeutic importance but when they get into the environment, especially water bodies, they become pollutant either directly or indirectly depending on their metabolites. This includes the excessive use of pharmaceutical agents, which creates serious problems when they find their ways into the environment. However, the currently used treatment techniques in most African countries were not designed to cater for these emerging contaminates. The performance of chemically modified vermiculite clay (VCM) and unmodified vermiculite clay (VCL) were evaluated for the removal of emerging pharmaceutical waste (4-aminoantipyrine) from aqueous solution. This was followed by development of guideline for handling wastewater in Nigeria. Currently, there are none. The chemical modification of VCL was achieved using cellulose nanocrystals (CNCs) and nitrilotriacetic acid (NTA) via facile dispersion and intercalation. After the modification, the BET surface area of VCL increased from 4 m2g-1 to 96 m2g-1 in VCM. The removal of 4-aminoantipyrine was pH dependent which followed pseudo-second-order kinetics. Langmuir isotherm model provided the best fit for the sorption data while a percentage removal of 4-aminoantipyrine unto VCM of up to 98.410 % was attained. Quantum chemical computational analysis was also used to describe the sorption process in molecular terms. The lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO) are distributed over the molecule of 4-aminoantipyrine and interaction between the surfaces of VCL/VCM and 4-aminoantipyrine may have occurred via donor-acceptor interactions. A regeneration capacity of 76 % was obtained for VCM while that of VCL was 60 %. Collation of previously generated data enhanced the development of guidelines for handling both domestic and industrial wastewater in Osun state, Nigeria. A discovery, which led to advocacy for water renewed policy for the people of Osun state, Nigeria. The study has revealed that the property of vermiculite clay can be improved via facile dispersion and intercalation with the potential of removing pharmaceutical pollutants from water system, which aids provision of water handling guidelines in Nigeria.

Abstract ID: 112

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Magnetism and Magnetic Materials

Keywords: Hall effect, electrical resistance, effective spin-orbital

The research of spin-orbital interaction in intermetallic compounds of system Tb-In on paramagnetic area

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An analysis of the experimental data demonstrates a correlation between the Hall coefficient RH and the magnetic susceptibility for the intermetallic Tb2In and Tb5In3 compounds shown in Fig. 1. As can be seen from the figure, the dependence of RH on is linear for the samples. Extrapolating RH to zero (OY axis), the normal, R0, and anomalous, RS, components of the Hall coefficients can be determined.

The normal, R0, and anomalous, RS, components of the Hall coefficient were determined from experimental investigations of temperature dependences of the Hall coefficient, magnetic susceptibility, and specific electrical resistance of the intermetallic Tb2In and Tb5In3 compounds.

Abstract ID: 113

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Novel Magnetic Materials and Device Applications

Keywords: Intermetallic YCo2; MgCu2-type structure, Exchange interactions, Magnetocaloric properties

Structural, magnetic and magnetocaloric properties of Co-Y-Cu compounds.

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We have investigated the effect of the substitution of the Cu atom by Y on the structural, magnetic and magnetocaloric behaviors of Co2Y1-xCux ($0 \leq x \leq 0.1$) compounds. We report on the synthesis of a series of Co2Y1-xCux ($0 \leq x \leq 0.1$) alloys and the investigation of their properties. Besides, the magnetic entropy change and the related Relative Cooling Power (RCP) values, sensitive to Cu doping, were estimated.

Abstract ID: 114

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: All solid-state batteries

Keywords: NCM cathode materiual, all-solid-state battery, energy storage

Tailoring NCM Cathode Materials for Application in All-Solid-State Batteries

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Bulk-type all-solid-state batteries (SSBs) are being considered as a viable next-generation energy storage technology, potentially offering both higher energy and power densities than state-of-the-art lithium-ion batteries. A promising materials combination for realizing SSBs consists of Ni-rich layered oxide cathode materials (CAMs), such as Li1+x(Ni1–y–zCoyMnz)1–xO2 (NCM), and lithium thiophosphate solid electrolytes (SEs) [1]. However, the occurrence of detrimental side reactions at the CAM/SE and/or conductive additive/SE interfaces (leading to performance decay) is a major obstacle toward commercialization of such SSB cells. Hence, a large part of research is devoted to CAM surface modification to inhibit interfacial side reactions (SE decomposition).

Apart from the need for a protective surface coating, we demonstrate the importance of tailoring NCM CAMs in terms of size/morphology and composition. Our research data indicate that such materials characteristics must be taken into account to improve the cell performance [2-4]. In particular, we show the influence of CAM size and composition both on the attainable capacity and on the internal pressure build-up upon cycling. Moreover, we will present our recent findings on the effect of CAM surface coating chemistry on the gas evolution in pelletized SSB cells [5].

Abstract ID: 115
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Bio-composites
Keywords: Molecular-imprinting, Ascorbic acid, Alginate Adsorption

Surface molecularly imprinted amino-functionalized alginate microspheres for enantio-selective extraction of L-ascorbic acid

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A surface molecular imprinting technique was utilized in the fabrication of an enantio-selective adsorbent based on amino-functionalized alginate microspheres for chiral resolution of ascorbic acid. Alginate microspheres were first strengthened via epichlorohydrin (ECH) covalent cross-linking then functionalized with amino groups through graft copolymerization of polyacrylamide (PAm) followed by Hofmann degradation. Surface molecular imprinting was then performed under mild conditions by ionic interaction between the surface incorporated amine groups and the template L-ascorbic acid enantiomers followed by cross-linking with glyoxal. L-Ascorbic acid enantio-selective adsorbent (LA-Alg) was finally obtained by removing the template molecules out of the cross-linked network formed on the surface of the modified alginate particles. The synthetic steps were monitored using elemental analysis and FTIR spectra. Also, the surface morphologies of the native unmodified alginate along with both imprinted and non-imprinted adsorbent particles were examined by SEM. Moreover, the crystalline profile and thermal properties of both native and modified samples were investigated using XRD spectra and thermogravimetric analysis (TGA), respectively. The effect of pH on the extraction process was studied and indicated that the maximum adsorption was obtained at pH 4. Also, adsorption isotherms over LAAlg adsorbent displayed the best fit with Langmuir model with maximum adsorption capacity 116 ± 1 and 67 ± 1 mg/g with respect to both L- and D-ascorbic acid, respectively. Moreover, the chiral resolution experiment using batch technique indicated 72% enantiomeric excess.

Abstract ID: 116

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Functionally graded composite materials and structures

Keywords: Compliant Mechanisms, Bistable Mechanisms, Curved Beam, Mechanical Behavior

Effect of Dimensional Parameters on the Mechanical Behavior of Curved Beam Bistable Mechanisms

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Compliant mechanisms (CM) are vastly studied due to its advantages, such as no need of lubrication, fewer parts and simple manufacturing. Bistable mechanisms (BM) are one of the many types of available CMs. One of the configurations of BMs is formed by connecting two beams at their center, which may be straight or curved beams. This way, a BM can be created and allow applications such as switches, valves, relays, positioners and mechanisms with shock isolation purposes. In this work, a mechanism with a pair of curved beams is used as a model to study the effect of the variation of curved beam parameters on the mechanical behavior of the mechanism. The beam span, apex height and side length were the chosen parameters to be varied, once they are the most relevant to the mechanism design. A comparison was made between the analytical mechanical behavior of the mechanism and numerical approaches, namely, chained beam constraint model (CBCM) and finite element analysis (FEA). It was observed that the side length of the mechanism has major relevance on the bistability condition and the apex height and beam span also play an important role in the force-displacement behavior.

Abstract ID: 117

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: degradation, photocatalyst, spectroscopic, 4-nitrophenol, TiO2

Synthesis of Ag–N–P-Tridoped TiO2 Nanocomposite Photo-catalyst for the Degradation of Organic Pollutants in Aqueous System

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Nanosize Ag–N–P-tridoped TiO2 composite photocatalyst has been prepared following sol–gel technique using commercial TiO2 and soybean (Glycine max)/ chickpea (Cicer arietinum) seeds as precursors. As-synthesized nanomaterial was characterized by XRD, FTIR and UV–visible spectroscopic techniques. Average crystallite size of the photo-catalyst material was within 30–45 nm. Whereas, doping Ag in TiO2 minimized the photo-generated electron–hole recombination, doped N and P extended its photo-absorption edge towards visible region. Tri-doping of Ag, N, and P in TiO2 exhibited synergetic effect toward enhancing the photo-catalytic degradation of 4-Nitrophenol pollutant in water. Using optimized reaction conditions, degradation of the pollutant, at three hours, were as high as 73.8 and 98.1%, under UV and visible irradiations, respectively. As the efficiency of the above photo-catalyst has proved very high under visible light, the same can be recommended for the cost-effective large scale treatment of water polluted with phenolic compounds.

Abstract ID: 118

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Carbon and metal oxide based composite materials

Keywords: Graphene Oxide, Steroid Estrogens, Biomass, Visible light, Photocatalyst, functional clay

CLAY-BASED HETEROJUNCTION IRON OXIDE-GRAPHENE OXIDE VISIBLE-LIGHT PHOTOCATALYSTS FOR THE REMOVAL OF STEROID ESTROGENS IN WATER.

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This study reports the development of visible light-mediated functional clay-based FeO-graphene oxide (GO) photocatalysts and their use in the removal of steroid estrogen from the water system. The aim is to make clean drinking water available in accordance with SDG 6. These steroid estrogens are potential causes of infertility in humans as well as diseases such as testicular, cervical and breast cancers. The photocatalysts were prepared from cheap and readily available materials (Kaolinite clay and Carica papaya seeds) via simple chemical reaction (conversion of waste to wealth). They were characterized by different techniques such as SEM, EDX, TEM, FTIR, BET, RAMAN, UV-DRS, PL, TGA, DTG and XRF. The Tauc plot bandgap for the photocatalysts ranged between 1.93 and 2.13eV with samples that contain GO having the lowest bandgap energies. Photocatalytic activity against steroid estrogens [Estrone (E1), 17-β estradiol (E2), estrone (E3) and 17-α ethynyl estradiol (EE2)] suggested a good photodegradation at >80% removal of all compounds under 720 mins. Photolysis and dark experiment (with photocatalyst) suggests far lesser results, which indicates the process is visible light-mediated photocatalysis. The efficiency of the FeO@PSK@GO was found to be the best of all the catalysts which further confirms what the result from the UV-DRS and PL which showed that the addition of graphene oxide increased the efficiency of the photocatalyst. The plausible degradation intermediate product of the steroids hormones were investigated by LC/MS analysis while the toxicity of the untreated and treated steroid estrogens solutions was evaluated using ceriodapnia silvestrii Spp and the LC 50 was evaluated for the steroid estrogens which showed to be 7.69, 6.56, 7.69, 6.70mg/l respectively; it also showed that the degraded effluent did not have any effect on the organisms. The COD experiment was also carried out to evaluate the level of mineralization of the degraded effluent and the results were as follows 57.16%, 65%, 68.80%, and 73.21% respectively for the different steroid hormones. The same treatment was applied to raw wastewater, rainwater and tap water from point-of-use mode; the result showed of which present functional clay photocatalyst as a potential solution for the removal of steroid hormones molecules from water.

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Abstract ID: 119

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: DFT, LAPW, Sb2S3 Thin Film, Solar Cell, Optical Properties

First-Principles Calculation of Optoelectronic properties of Antimony Sulfides Thin Film

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Antimony sulfide (Sb2S3) thin film have received great interest as an absorbing layer for solar cell technology. Electronic and optical properties of Sb2S3 thin films were studied by first principles approach. Highly accurate full-potential linearized augmented plane wave (FP-LAPW) method within the framework of density functional theory (DFT) as implemented in WIEN2k package. The simulated film is in the [001] direction using supercell method with a vacuum along z-direction so that slab and periodic images can be treated independently. The calculated values of indirect band gaps of Sb2S3 for various slabs were found to be 0.568, 0.596 and 0.609 eV for 1, 2 and 4 slabs respectively. This trend is consistent with the experimental work where the band gap reduced when the thickness increased. Optical properties comprising of real and imaginary parts of complex dielectric function, absorption coefficient, refractive index was also investigated to understand the optical behavior of Sb2S3 thin films. From analysis of optical properties, it is clearly shown that Sb2S3 thin films have good optical absorption in the visible light and ultraviolet wavelengths, it is anticipated that these films can be used as an absorbing layer for solar cell and optoelectronic devices

Abstract ID: 120

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Bio-inspired design of composites

Keywords: E-skins, Fingerprint, Selective Perception

The Design, Mechanism and Application of Novel Sensing Materials and Structure for Selective Perception of Prosthetic Hand

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Nowadays, the flexible sensors called e-skins are constructed to mimic the skin of human beings for acquiring perceiving outside force information, which is of great significance to bionic applications, such as neuroprosthetics and robotics. However, the reported sensors mainly focus on the detection of normal force or hybrid pressure but lack of the capacity of measuring or distinguishing non-normal sheer force directly. Inspired by the spiral structure and Ruffini endings functions of fingerprint, we demonstrate a tangential force sensor to imitate multiple functions of hand skins based on capacitance sensing technology, which is able to selectively detect static friction and sliding friction force in real time. The capacitance of the as-obtained sensor keeps constant when applied normal force, decreases when applied sliding friction force and increases when sliding occurs. And we also demonstrate that this ability of specific response to static friction and sliding friction force in real time can be used to recognize sliding and object weight for robotic hands, which can help robots and prosthetic hands to do more complex tasks. Besides, we also achieve the signal encoding by the designed circuits. That is, the capacitance signals are transferred to the bionic pulsed signal and the frequency of pulsed signals is higher during sliding process, which is meaningful for expanding the sensing ability of neuroprosthetics.

Abstract ID: 121

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Bio-inspired design of composites

Keywords: Wettability, Nano, Bioinspired.

Bioinspired surfaces with micro- and nanostructures: from design to functions on dynamic wettability

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Natural biological surfaces (e.g., spider silk, cactus spine, butterfly wing, lotus leaf, etc.) have inspired us to design the functional materials and surfaces [1-3]. Inspired by the structures of biological surfaces and materials, some bioinspired gradient surfaces have been designed by integrating physics-chemistry methods, e.g., dip-coating, Rayleigh instability break-droplets, electrospinning, and wet-assembly, etc.. The gradient features can be including in roughness and curvature, gradient spindle-knots, star-shape wettable pattern, etc. For instance, the surfaces and materials with the conical spines andperiodic roughness or micro- and nanostructures can achieve the high-efficiency condensed-droplet transport. In addition, some photo-thermal organogel surfaces for controlling of droplet transport in various routes via light radiation; Magnetic-induced dynamic tilt-angle pillar array for driving of the droplet shedding-off in directions. These bioinspired gradient surfaces exhibit robust transport and controlling of droplets. These studying would be significant to design the novel engineering surface and materials for promising applications such as anti-icing, liquid transport, anti-fogging/self-cleaning, water harvesting, etc.[1-3]

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Abstract ID: 122

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Montmorillonite, titania pillared clay, ceramic membrane, photocatalysis, methylene blue

Synthesis and Characterization of Titania Pillared Clay Membranes for Methylene Blue degradation in Textile Wastewater

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Textile effluent contains dyes in the range of 50-1000 ppm and at low concentration of 10-50 ppm, thus producing intense colour. According to the Environment Protection Act, these toxic wastes are called ‘emerging pollutants’ which cannot be degraded by any means. Titania photocatalyst is widely used for degradation of contaminants in wastewater, but its usage suffers from many drawbacks like its ease of separation from the suspension and its tendency towards forming agglomerates which reduces its photocatalytic activity. Amphoteric membranes such as Titania pillared clay membranes exhibit different charges at different pH values, subsequently show efficient separation for cationic and anionic pollutants in wastewater based on solution pH. The structural properties of such membranes determine their permeability and selectivity to a large extent. The present work is envisaged to synthesize TiPILC membranes by immobilizing titania on clay support and further sintered at different temperatures 300degC, 500degC, and 600degC. X-Ray Diffractograms of the membrane material sintered at these temperatures reveal the presence of a mixture of phases, anatase and brookite, responsible for enhanced photocatalysis. Fourier Transform Infra-Red spectra reveal complete intercalation of Ti4+ ions into interlayer spaces of clay leading to a homogenous material. Brunauer Emmett Teller specific surface area study reveals a narrow pore size distribution curve which reflects the selectivity of the membrane surface. Such a ceramic membrane reactor, an integration of separation along with photocatalysis, when treated with Methylene Blue dye resulted in its ~99% decolourisation in just two cycles of the filtration process.

Abstract ID: 123
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Ceramic based composites
Keywords: flexible piezoelectric, organic-inorganic hybrid, BaTiO3, wearable sensor

Flexible and Ultrasensitive Piezoelectric Composites Based on Highly (00l)-Assembled BaTiO3 Microplatelets for Wearable Electronics Application

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Piezoelectric wearable electronics with flexibility and high sensitivity has received increasing attention in the fields of health monitoring, flexible robots and artificial intelligence. In this paper, a flexible organic-inorganic hybrid composite for wearable electronics application based on (00l)-aligned BaTiO3 (BT) single-crystal microplatelets was prepared by Layer-by-Layer self-assembly technology. For the polyvinylidene fluoride-trifluoroethylene (P(VDF-TrFE))/BT single-crystal microplatelets composite film, the sensitivity is nearly 20 times higher than that of its counterparts of P(VDF-TrFE)/BT microparticles composite film and pure P(VDF-TrFE) film. The orderly alignment of BT microplatelets also has been found advantageous to the strength of the composite film. The tensile strength is up to 204.3MPa even at a high inorganic phase content of 53.8wt% in P(VDF-TrFE)/BT single-crystal microplatelets composite film, which is four times as that of pure P(VDF-TrFE) film. Moreover, the flexible piezoelectric wearable device based on P(VDF-TrFE)/BT single-crystal microplatelets film effectively provides detailed information for monitoring human activities such as pronunciation, frequency and waveform of pulse beating, and motion states. This high sensitivity, high strength and flexible piezoelectric composite provides much potential on the applications of wearable equipments and health monitoring devices.

Abstract ID: 124
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Bio-composites
Keywords: Bio-based, thermosets, composites, cellulose.

Natural fibers bio-based thermoset composites as substitutes for industrial petro-based matrices with synthetic fibers composites

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In recent years, due to the uncertainty of the cost and supply of petrochemicals, large amount of research and development has been made to develop safer, and more sustainable materials with a high weight/strength ratio. Thermosetting resins and thermoset composites once formed and cured are highly cross-linked, cannot be remolded, reshaped, or reformed. The higher flexibility for tailoring desired ultimate and high-performance products for industry leads to its strength, better thermal and chemical resistances. Composite materials are used a wide range of application because of their low weight and excellent properties, enabling the production of lighter weight materials. Nowadays, most thermosets resins are petro-based. Epoxy and vinyl-ester resins which are commonly used in the industry are derived from bisphenol-A(BPA). BPA have been proven proved to be a reprotoxic substance. Moreover, composites production generally employs volatile organic compound (VOC) such as styrene to reduce the resin viscosity and enable liquid molding, but hazardous air pollutant (HAP) are produced during curing. Synthetic fibers such as glass fiber a high energy demanding to produce and prevent industrial composites recyclability. Therefore, and due to increasing environmental concerns, access to bio-based and non-harmful materials for industrial applications is needed. Natural fiber reinforced polymer composites (NFPC) have gained considerable attention in the recent years due to their environment and economic benefits, beside low energy consumption during production. Cellulose is an abundant, renewable and biodegradable naturally occurring material on earth that can be obtained from biomass. Here in, a styrene-free cardanol-based vinyl-ester resin was used as a substitute for polyester and vinyl-ester commercial resin. The thermoset resins studied herein were coupled with cellulose microfibrils (Provided by Kruger Inc.) as a substitute for synthetic glass fiber to produced thermosets composites. Rheological, thermal and mechanical properties of both synthetic and bio-based materials were investigated by scanning electron microscopy, DSC, TGA, and tensile tests. These results indicate that cellulose microfibrils, exhibit excellent reinforcement effect on the matrices, and appeared as a promising substitute for glass fiber as a filler or woven for structural, automotive, construction and electronics applications. Moreover cardanol-based materials produce herein demonstrate that safer alternative thermosets resin may be produced from biomass at a semi-pilot scale for composites applications.

Abstract ID: 125

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Fiber reinforced Composites

Keywords: Fiber reinforced composite, porous composite, natural fiber, acoustic material, noise reduction

Cost-Effective and Environment Friendly Acoustic Materials from Natural Fiber based Porous Polymer Composites

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Porous polymer composites are getting increased attention as better acoustic materials. The incorporation of natural fiber as reinforcement and sound absorption strategy in these systems can be beneficial in replacing the glass wool which is hazardous in making the composites environment friendly. In the present study natural plant fiber based polymer composites were synthesized with varying fiber content, incorporation of sound resonators, design strategies to produce cost-effective and non-hazardous acoustic protecting materials for building industry. The flammability, density and thickness of the tiles were optimized for better noise reduction coefficient and sound absorption compared to commercial glass wool based panels. The results showed a novel route for effective acoustic protection utilizing designer tiles of low density porous polymer composites with natural fibers which are comparatively cost-effective compared to glass fibers.

Abstract ID: 126

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Optical properties of metals and non-metals

Keywords: Hybrid nanoparticles, tunable emission, photon upconversion, energy transfer

Lanthanide based hybrid nanostructures: Multicolour luminescence, energy transfer and multifunctional applications

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We have synthesized a rare-earth based novel inorganic-organic hybrid nanostructure (IOHN) composed of fluoride nanophosphors and β-diketones coordination compounds.[1-3] The fluoride nanophosphors separately give intense emission in visible region under near infrared (NIR) excitation, known as upconversion (UC) emission, while β-diketones coordination compounds again give intense emission upon ultra-violet (UV) excitation, known as downshifting emission. The IOHN, therefore, gives intense emission upon both UV and NIR excitation sources. The XRD and FTIR measurements reveal both the systems are not bonded with each-other, rather entangled with weak interacting forces. The TEM analyses reveal that, the prepared ultrafine upconversion nanoparticles are dispersed on the surface of coordination compounds. The IOHN comprises excellent dual-mode optical features (DS and UC) of both the phases. Energy transfer from Er3+/Ho3+ (doped in inorganic phase) to Eu3+/Tb3+ (coordinated in organic phase) demonstrates for a viable coupling between both the phases. Because of ultrafine particle size the surface to volume ratio is relatively higher which improves the attachment of particles with the fingermarks. To further enhance the dual mode emission of IOHN, Silver nanoparticles (AgNPs) have been introduced. The emission intensity of UC as well as DS emission has been found to be strongly modulated in the presence of AgNPs. It has been found that AgNPs enhances UC emission. The excellent optical properties of these nano-hybrid materials provide a great opportunity in the field of ultraviolet (UV) sensing and energy devices.

Abstract ID: 127
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Bio-composites
Keywords: Thermoelasticity, Human head, Skin, Bone, Brain, cellular devices

Generalized Thermoelasticity of Multi-Layer Human Head Subjected to Electromagnetic Energy Due to the Cellular Devices

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In this work, a mathematical model of the human head consists of three layers skin, bone, and the brain has been constructed. The internal thermal reaction-generated through the human head due to the chemical reactions of the tissue has been considered with the phase-lag-time definition to stand on the response time of the three layers takes due to the perturbation. The governing equations have been introduced in the context of the generalized thermoelasticity model based on non-Fourier law of heat conduction. The techniques of the Laplace transforms will be used, and its inversions will be calculated numerically by using Tzou method. The temperature increment, the displacement, the stress, and the deformation distributions will studied through the three layers of the human head with various values of time, depth, relaxation time, frequency of power transmission, and power density when the human is subjected to an electromagnetic wave due to cellular devices.

Abstract ID: 128

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: 2D materials, meso-entropy matter, high-entropy isomer, graphene, carbon, topological defect

Meso-Entropy Materials: From PAH Isomers to Topological Defect of Graphene

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In the past decades, various materials have been developed, especially for carbon-rich materials. The most popular carbon-rich materials include fullerene, carbon nanotube, graphene, graphite, diamond, and polycyclic aromatic hydrocarbons (PAHs). Although studies appear to be exhaustive, the relationship between these materials remains unclear. Even for one of them, the understanding at chemistry level is still at the stage of hybridization difference. In this talk, I'd like to propose a new method, the meso-entropy concept, to re-understand carbon materials and forecast new carbon-rich materials with new properties.

Abstract ID: 129

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Smart Composites

Keywords: Carbon fibers, Conductive mortar, Electrical resistivity, Dielectric properties, Multifunctional concrete, Self-sensing material

Self Sensing Cement-based composites with Short Carbon Fibers

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This paper is aimed at exploring mechanical, electrical and self-sensing properties of cement-based mortars through the addition of short carbon fibers, at different dosages (2%, 3%, 4% by weight of cement). Compression and bending tests on carbon fiber reinforced cement-based materials (CFRCM) were performed. The addition of carbon fibers showed to enhance the mortars' flexural strength by increasing the fibers content, while no improvement was found in the compressive strength. Electrical resistivity of the CFRCM, at different days of curing, was evaluated by AC impedance measurements, using two stainless steel wire meshes as electrodes. The electrical resistivity decreased with time, until reaching a constant value after about 60 days of curing. Carbon fibers were able to drastically reduce the mortar resistivity, up to values below 150 Ω cm. The effect of fibers dosage on the ability of the mortar to change its electrical resistivity when subjected to different stress states was also studied. The specimens were gradually loaded up to 50–60% of the maximum compressive strength, carrying out two loading/unloading cycles, while resistivity was measured using a conductivity meter. Depending on the fibers dosage and stress state within the material, CFRCM resistivity changed with significant variations.

Abstract ID: 130

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Electrochemical properties of graphene, Mxenes and other two-dimensional materials

Keywords: Graphene Quantum Dots, 2D Materials, Oxygen Evolution Reaction

Atomically Dispersed N-Graphene Quantum Dots-Supported Dinitrosyl Iron Catalyst for Superior Oxygen Evolution Reaction

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The development of robust and non-precious electrocatalysts with high catalytic activity is broadly desired for fuel cell commercialization. Here, we report an electrocatalyst of dispersed Fe(NO)2 moiety anchored to nitrogen-doped graphene quantum dots (N-GQDs) to form a N-GQDs-Fe(NO)2 complex that shows a superior oxygen evolution reaction (OER) with a Tafel slope of 47 mV/dec, which exceeds the state-of-the-art RuO2 (82 mV/dec). Combining X-ray photoelectron spectroscopy and scanning transmission electron microscopy-energy dispersive spectrometer mapping results revealed the catalytically active sites to be monodispersed N-GQDs-Fe(NO)2 complex that maintain their oxidation state during OER, probably via electronic coupling to the conductive graphene support. Electrochemical data suggest that the Fe-N-C configurations derive their excellent activity from faster OH- adsorption than that of conventional N-C configuration sites. These unique properties of N-GQDs-Fe(NO)2 complex electrocatalyst could offer a facile route to fabricate non-precious and high OER active electrocatalysts for clean energy applications.

Abstract ID: 131
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Multifunctional composites
Keywords: Fibrous mesoporous silica, Adsorption, Hierarhical porous, Formation mechanism, N-doped carbon microspheres

Fibrous N-doped Hierarchical Porous Carbon Microspheres: Synthesis and Adsorption Performance

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The creation of high surface area and effective active sites is the key problem for the synthesis of high-performance porous carbon materials. In this work, polyacrylonitrile-coated fibrous silica (F-SiO@PAN) microspheres were prepared by in situ polymerization of acrylonitrile on fibrous mesoporous silica microspheres induced by γ-ray radiation. After F-SiO@PAN microspheres were carbonized and etched with hydrofluoric acid, uniform fibrous N-doped porous carbon (FNC) microspheres with an average size of 286 nm and a molar ratio of C/N of 5.2 were successfully prepared. As revealed by TEM, SEM, and N adsorption-desorption isotherms analysis, FNC microspheres have a hierarchal micro-macroporous structure with a particular high surface area of 554.5 m2/g. The FNC microspheres also exhibit a good water dispersibility and an excellent adsorption ability to rhodamine B in water. The equilibrium adsorption capacity of FNC microspheres could reach 95.4 mg/g, which is 1.6 times as that of the primary silica template microspheres. The adsorption kinetics and thermodynamics of FNC microspheres are in accord with the pseudo-second-order kinetic equation and Freundlich isotherm model, respectively. This work provides a facile synthesis method for novel N-doped hierarchical micro-macroporous carbon microsphere as a potential high performance adsorbent material.

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Abstract ID: 132

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Magnetism and Magnetic Materials

Keywords: Manganites, Temperature coefficient of resistance, Magnetoresistance

Enhancement of magnetoresistance (MR) and temperature coefficient of resistance (TCR) of La0.67-xRExCa0.33MnO3 (x = 0, 0.1; RE = Gd, Nd, Sm) system via rare-earth substitution

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Among all the perovskite manganites, the calcium-doped La0.67Ca0.33MnO3 (LCMO) compound has been studied extensively due to their high-temperature coefficient of resistance (TCR) and magnetoresistance (MR) [1,2]. This study offers a promising route to greatly enhance the temperature coefficient of resistance (TCR) and magnetoresistance (MR) of rare-earthed doped LCMO system for possible applications. We have investigated the influence of rare-earth doping on structural, electrical, magnetic, and thermal properties of La0.67Ca0.33MnO3 compound. The Rietveld refinement of the X-ray data confirms that the doped RE (RE = Nd, Sm, and Gd) elements partially substitute the La site. It is also observed that RE doping at La site changes the Mn-O bond length and Mn-O-Mn angles, but the structure of the compound remains unchanged. The metal-insulator transition temperature decreased with the decrease in the RE ionic radii. The high-temperature resistivity can be explained reasonably well by the small polaron hopping model. The phenomenological percolation model could reproduce the resistivity data in the entire temperature range, suggesting the segregation of ferromagnetic metallic clusters and paramagnetic insulating regions. The analyses of the Seebeck coefficient data reveal that the mechanism of high-temperature thermoelectric transport is due to the small polaron hopping, whereas the electron–magnon scattering plays the dominating role at low temperatures. Thermal conductivity is found to decrease with decreasing the ionic radii of dopant, indicating the destabilization of Jahn-Teller distortion. Most importantly, the TCR and MR enhance significantly with rare-earth doping in the La0.67Ca0.33MnO3 system.

Abstract ID: 133

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Concrete and cementitious composites

Keywords: FRP, Reactive Powder Concrete, Composite beam, flexural strength, plastic-damage model

Experimental Study and Simulation of Flexural Behavior of FRP-RPC Composite Beam

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Strengthening of concrete members by using fiber reinforced plastic (FRP) has emerged as a viable technique to enhance their ductility and deformation tolerance. Reactive Powder Concrete (RPC) is an ultra-high-strength and high ductility cementitious composite material with excellent mechanical properties compared to ordinary concrete. FRP may be used as a permanent formwork of RPC members to enhance its flexural strength as traditional longitudinal rebars. In this study, the flexural test and simulation are carried out to investigate the flexural performance of RPC beams strengthened with FRP plates. In addition, different bonding treatment between RPC and FRP plates are also involved. The test results show that the ultimate flexural strengths of RPC beams increase from 33kN to 133kN with strengthened by FRP plates. This study also proposes an analytical model to predict the behavior of RPC-FRC composite beams. The surface-based cohesive behavior is also captured to represent the interfacial bonding between RPC and FRP. The numerical simulation shows an excellent agreement with the test results.

Abstract ID: 134

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Materials Integration

Keywords: Analytical Modeling, Electronic Materials, Photonic Materials, Physical Design for Reliability, Accelerated Testing

Application of analytical modeling in probabilistic design for reliability of electronic and photonic materials, assemblies, packages and systems

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Merits, attributes and challenges associated with the application of analytical ("mathematical") predictive modeling in electronics and photonics materials science and engineering are addressed. It is shown that application of analytical modeling enables revealing and explaining the underlying physics associated with often non-obvious, always non-trivial and in some cases even paradoxical, problems. Some of the addressed problems are: interfacial thermal stresses in adhesively bonded or soldered assemblies and application of inhomogeneous attachments for lower thermal stresses [1,2]; thermal and lattice mismatch stresses in semiconductor crystal grown assemblies [3,4]; dynamic response of electronic systems to shocks and vibrations [5,6]; stress relief in solder joints owing to their elevated stand-off heights and inhomogeneous solder joint systems for lower thermal stresses [7,8]; stress relief in thermoelectric module designs [9,10]; low-temperature micro-bending of long-haul dual-coated optical fibers [11]; two-point bending of optical fiber specimens [12,13]. It is concluded that analytical modeling occupies a special place owing to its ability to provide clear and concise information of the problems it addresses. The general concepts are illustrated by practical numerical examples.

Key Words: Analytical Modeling, Electronic Materials, Photonic Materials, Physical Design for Reliability, Accelerated Testing

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Abstract ID: 135

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Sensors, Composite materials, Nanomaterials, Thin films

Elastic waves and electron-phonon heat flow in nanocomposite thin films

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We consider an ultrathin metal layer deposited on an insulating membrane - a setup applied in ultrasensitive nanosensors, calorimeters, bolometers, electronic on-chip microcoolers [1]. When external energy is absorbed in such nanocomposite structure the effective temperature of the electron gas in metal rises above that of lattice vibrations (phonons) resulting in a heat flux between the two subsystems. Understanding this process is of vital importance for optimization of the device performance. Experimental studies have registered a dramatic change below a thickness dependent temperature T* in the power density of heat transfer which increases orders of magnitude in thin films compared to bulk materials while its temperature variation weakens [2,3]. It is shown that this behavior is due to dimensional crossover in the phonon spectrum which strongly modifies the electron-phonon coupling below T* [4]. The description accounts for the deformation potential interaction with acoustic modes. A complete analytic solution for the long wavelength region of their spectrum reveals some non-trivial properties of the elastic wave propagation in composite nanostructures [5]. In particular, acoustic properties depend on material parameters of the added or coating layer in a strongly non-monotonous way. Thus, for the lowest energy mode (flexural wave) increasing the layer thickness may lead to a sharp increase and then a sharp drop of the phase velocity with a similar unusual pattern being reflected in the electron-phonon heat flow, also observed experimentally. It is found that amplitudes of the elastic vibration modes have a topological characteristic related to their signs on the surfaces of the free standing or suspended composite structure, i.e., they demonstrate stability with respect to “deformation” (variation) of the material parameters (elastic moduli, mass densities, thicknesses). It is also shown how the lowest energy branches of the spectrum are connected to the surface and interface guided waves (Rayleigh and Stoneley) at shorter wavelengths.

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Abstract ID: 136

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Dielectric, Ferroelectric and Piezoelectric materials

Keywords: Nanodielectric, Capacitive Energy Storage, High temperature, Film capacitor

Nanodielectrics for High-Temperature Capacitive Energy Storage

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Polymeric dielectric materials enable film capacitor technology that is critical in high-power energy storage and pulsed power systems, hybrid electric vehicles, aerospace power conditioning and advanced electromagnetic weapons. Conventional high-temperature polymeric dielectric materials dissipate a large amount of heat as they are involved in continuous operations under high temperature and strong electric field conditions, which, unfortunately, leads to thermal runaway and failure of film capacitors. We propose to tackle the key issues associated with thermal runaway in plastic film capacitors by focusing on the suppression of charge injection from electrodes and thermally activated migration of charge carriers, rather than following the traditional design of high-temperature polymer dielectrics that only concerns the thermal stability of materials. Advanced composite approaches, thin-film deposition technologies, comprehensive characterizations of dielectric and capacitive energy storage properties as well as computational simulations are utilized to cover from structure control to material preparation, to performance assessment and to device modeling. The ultimate goal of this study is to develop novel high-temperature polymer dielectrics that can maintain dielectric stability and energy storage properties under high electric field and high temperature, and effectively suppress the thermal runaway of plastic film capacitors.

Abstract ID: 137
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Carbon/Carbon Composites
Keywords: Lightning, Carbon Fiber Reinforced Polymer Matrix Composite, Impulse Current Generator, Carbon Black, Carbon Nano Tube

Effect of Carbon Nano-Fillers on Improving the Lightning Strike Damage on Carbon Fiber Reinforced Polymer (CFRP) Composite Laminate

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Aerospace industry is highly interested in using Carbon Fiber Reinforced Polymer (CFRP) matrix composite laminates owing to its excellent properties, such as corrosion resistivity, light weight, low coefficient of thermal expansion, and high mechanical strength. CFRP composite laminates have become a promising alternative for conventional metallic parts in various applications. The most significant shortcomings of CFRP composite laminates are being flammable and having low conductivity which leads to damage and delamination of composite laminates when subjected to lightning strikes. The damage of CFRP composite laminate is attributed to the low electrical conductivity of the matrix which is usually a dielectric resin such as epoxy. Epoxy resin is one the materials that adheres to the carbon fiber effectively and contributes to strength, durability, and protection. A meticulous investigation on the material damage caused by a lightning strike impact is necessary to reduce the lightning strike damage of the CFRP composite laminates without deteriorating the mechanical properties. There have been numerous studies reported in the literature that added nano-fillers to epoxy resin for increasing the mechanical property and reducing the electrical resistivity of CFRP composite laminates, but the impact of adding nano-fillers on the lightning strike damage has not been systematically investigated. Graphene, carbon nanotubes (CNT), graphite, and fullerene are the carbon-based nano-fillers which are for polymeric materials.

The aim of this research study is to find out the correlation between damage on composite structures due to the lightning strike and the additive nano-fillers to the resin, while maintaining the original mechanical properties. CNT and Carbon Black (CB) are used to be dispersed in the epoxy matrix to create a better structure. The use of both CNT and CB makes a strong 3D network configuration in the matrix due to the CNT structure, where CB acts as a filler between CNT particles that leads to further enhancement in electrical conductivity and mechanical strength. In this regard, the lightning impulse current generator at our High Voltage Lab at Mississippi State University is used to generate component A of natural lightning phenomena in agreement with the Society of Automotive Engineers (SAE) standard. Our impulse current generator is capable of the generating various lightning impulse currents with the amplitude as high as 200 kA. Different amounts of CNT and CB are added to the epoxy resin, and the damage mode on CFRP composites such as delamination, fiber pullout, and charring are visually analyzed after lightning strike by Scanning Electron Microscopy (SEM) to identify the effect of adding nano-fillers. The outcome of this paper contributes to reduce the lightning strike damage on CFRP composite laminates.

Abstract ID: 138
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Bio-composites
Keywords: Polymer composites, dental composites, dental resins, close packing.

Design and Formulation of New Dental Resin Composites

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Dental polymer composites are composed of hard, finely ground filler particles, surrounded by a photo-polymerizable organic matrix which binds the filler particles together like a glue. The composite materials are preferred since they are more esthetic than mercury amalgam with a dark color. The inorganic filler particles in dental resin composites serve to improve their mechanical and wear properties and reduce polymerization shrinkage during their use. To achieve improved mechanical and wear properties of these composites, it is important to increase and optimize the inorganic filler contents in the composite.

The theory of close-packed structures of spherical particles was used for the refinement of filler formulations with the aim to estimate the maximum allowable loading of the particles. We demonstrated that the theoretical estimation of mixtures of spherical particles of different sizes is used to serve as a guideline in the design and formulation of new dental resin composites with better properties and improved performance. We have also made wrinkled silica fillers to improve the resin composites, including viscosity, optical and mechanical properties. The new materials are potentially useful in hard-tissue engineering such as tooth, bone and cartilage restoration for medical purposes.

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Abstract ID: 139
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Bio-inspired design of composites
Keywords: Lipid-A phosphate, self-assembly, phases, non-equilibrium transitions

Non-equilibrium lipid-A phosphate phases against bacterial and aniviral infections

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Lipid A-diphosphate is the abundant component of bacterial lipopolysaccharides (LPS) and found on the surface of Gram-negative bacteria outer membrane. The commensal microbiota effects the mucosal and systemic immunity, playing a potential role for microbial keystone species in autoimmunity, and rely on autonomous natural components1 to sense their surroundings due to the variation in LPS pattern and nosocomial infections. The resistance to common administered antibiotics has resulted in a growing interest in therapies using non-toxic lipid A-phosphate or their approximants. Lipid A-phosphate and/or approximants self-assembled into body-centered and face-centered cubic liquid crystals2. However, lipid A-phosphate phases driven out of equilibrium, particularly those in complex with lipid A-derivatives exhibit new structures with different properties and antimicrobial responsiveness than those at equilibrium. The crystalline phase and the liquid phase, the lipid A-diphosphate molecules exhibited two non-equilibrium phases with various degrees of translational and orientational order. A transition of lipid A-diphosphates is observed between phase-separated-fatty-acid chains and a mixed honeycomb non-equilibrium phase. The development of different 2-d faceted crystal morphologies was observed and, as growth proceeded, these faceted 2-d crystals became unstable and self-organize far from thermal equilibrium. The 2-d crystalline lipid A-diphosphate layers exhibited a pseudo-hexagonal molecular arrangement3. The development of these specific antagonistic structures creates and eliminates antimicrobial resistance, or disease-related events to booster the host defense against pathogenic invaders. For lipid A-monophosphate, rhombodo-decadecahedra (Fd3m) packing was suppressed because of instability in the mean curvature between the tetrahedral and the octahedral nodes. Tetrakaidodecahedra packing showed only tetrahedral nodes; the tetrahedral angle could only be retained between all edges if the hexagonal faces of the truncated octahedron were changed. The (Fd3m) multidomain structure with identical lipid A of 30°- rotated and - unrotated none-endotoxic lipid A-diphosphate layers resulted in diffraction patterns that show 12-fold rotational symmetry in the diagonal direction, for those complexes with non-identical lipid A but antagonistic lipid A-diphosphate. The spatial packing of these “spheres” was either a cuboctahedron or an icosahedron4, interesting samples of rhombohedral traps for oligomerization in membranes5.

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Abstract ID: 140

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Functionally graded composite materials and structures

Keywords: Functionally Graded Materials, Buckling, Finite Element Analysis, Partial Edge Loads, Plates

Buckling of Functionally Graded Plates Subjected to Partially Distributed Edge Loads

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Buckling behaviour of Functionally Graded Material (FGM) plates subjected to various partially distributed in-plane compressive edge loading is studied using finite element analysis (FEA). The effective material properties of the FGM plates are assumed to vary in the thickness direction according to power-law distribution of volume fraction of the constituents. As the initial pre-buckling stress distribution is nonuniform in nature for a given loading and edge condition, the critical loads are calculated by the dynamic approach. In this study first-order shear deformation theory is used to model functionally graded material plates, considering the effect of transverse shear deformation. Towards this, the plate is discretized by using an eight noded iso-parametric plate element with five degrees of freedom at each node. The analysis is carried out for four types of partially distributed uniform edge compression load, viz., (i) Concentrated edge load from the corner (ii) Partial edge loading at the centre (iii) Partial edge loads from both the ends and (iv) Partial edge load from one end. Convergence and comparison studies have been performed to describe the efficiency of the present model. Solutions obtained from finite element analysis are first validated with results available in the literature for isotropic plates subjected to uniaxial concentrated and partially distributed edge compression loads. Effect of different parameters such as volume fraction index, boundary conditions, modular ratio, side to thickness ratio (b/h), percentage of loaded edge length and edge ratio (a/b) of the plate are considered to study the buckling behaviour of the plate. From the current studies it is concluded that the buckling strength of the functionally graded plate is highly influenced by partially distributed edge loads as compared to plates subjected to uniformly distributed full edge compression. With the increase in the edge ratio, the influence of partially distributed edge load on plate buckling load decreases.

Abstract ID: 141

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Solar Cells

Keywords: Flexible solar cell, organic photovoltaics, green solvent

Development of flexible semiconductor polymer solar cell capable of environment-friendly process by improving solubility using random arrangement of donor-acceptor structure

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In this study, thiophene units are introduced into the backbone of a semiconducting polymer in either a regular (PffBT-T4) or a random (PffBT-RT4) manner to determine whether the resulting semiconducting polymers are suitable for developing efficient polymer solar cells. PffBT-RT4 has lower crystallinity than PffBT-T4 due to its random configuration. Microstructural analyses indicate that PffBT-RT4 exhibits a shorter π– π stacking distance than PffBT-T4. Since short π–π stacking distance benefits inter-chain charge transport, PffBT-RT4 shows higher space-charge-limited current mobility, and PffBT-RT4 solar cells exhibit higher power conversion efficiency (PCE; 8.84%) than their PffBT-T4 counterparts (7.25%). In addition, PffBT-RT4 solar cells with active layers, prepared using a green solvent without any additive, show an encouraging PCE of 7.23%. Moreover, flexible solar cells based on PffBT-RT4 are much more stable during bending cycles than PffBT-T4 flexible solar cells. Therefore, this study demonstrates that the random configuration approach is a promising design strategy to realize semiconducting polymers for efficient, green-solvent processable flexible polymer solar cells

Abstract ID: 142

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Solar Cells

Keywords: crosslinking, organic photovoltaics, nonfullerene acceptors

Thermally stable ternary blended organic photovoltaics using green-solvent processable asymmetric semiconducting polymers capable of cross-linking

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The synthesized P2FBTT-Br can be crosslinked by UV irradiation for 150 s and dissolved in 2-methylanisole due to its asymmetric structure. In OPV performance and burn-in loss tests performed at 75 °C or AM 1.5G sun illumination for 90 h, UV-crosslinked devices with PC71BM show 9.2% of power conversion efficiency (PCE) and better stability against burn-in loss than pristine devices. The frozen morphology resulting from the crosslinking prevents lateral crystallization and aggregation related to morphological degradation. When IEICO-4F is introduced in place of a fullerene-based acceptor, the burn-in loss due to thermal aging and light soaking is dramatically suppressed because of the frozen morphology and high miscibility of the nonfullerene acceptor (18.7% □ 90.8% after 90 h at 75°C and 37.9% □ 77.5% after 90 h at AM 1.5G). The resulting crosslinked device shows 9.4% of PCE (9.8% in chlorobenzene), which is the highest value reported to date for crosslinked active materials, in the first green processing approach.

Abstract ID: 143

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Solar Cells

Keywords: Flexible all-polymer solar cell, Fluorination, Morphology, n-type conjugated polymer

Flexible All-Polymer Solar Cells with Improved Mechanical Stability and Photovoltaic Performance via Controlling Intermolecular Interactions

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Naphthalene diimide (NDI)-based copolymers have been highlighted as polymer acceptors in all-polymer solar cells (all-PSCs), but their large crystal domains cause large-scale phase separation in all-polymer blend films. This behavior inhibits the photovoltaic performance and mechanical stability of all-PSCs. Herein, all-polymer blend films were controlled by introducing a fluorinated copolymer of NDI and (E)-1,2-bis(3-fluorothiophen-2-yl)ethene (FTVT) (PNDI-FTVT) as a polymer acceptor for flexible all-PSCs. The copolymer PNDI-FTVT has a less crystalline structure and higher electron mobility than its nonfluorinated copolymer counterpart (PNDI-TVT). A blended film incorporating PNDI-FTVT exhibits a well-mixed morphology and improves the chain interconnectivity with a polymer donor, providing better charge transport pathways and enhanced mechanical resilience. The PNDI-FTVT based flexible all-PSC exhibits enhanced photovoltaic performance in comparison with a PNDI-TVT-based flexible all-PSC (5.11–7.14%) as well as excellent mechanical stability in a flexible all-PSC (7.14–5.78%), maintaining 81% of its initial performance at a bending radius of 8.0 mm after 1000 bending cycles.

Abstract ID: 144

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Experimental methods for Composite materials

Keywords: Carbon, fiber, 3D printing, sensor

1D and 2D Nanocarbon Alignment for Multifunctional Composites

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Nanoparticle alignment can benefit mechanical stress transfer, electron or photon transport, targeted drug delivery, enhanced Raman signals, among many other applications. Currently used methods such as electrical or magnetic fields are limited due to the requirement of responsiveness of nanoparticles, thus significantly limited the choices of materials that can be used in structural or functional composites. This talk will cover two novel manufacturing methods that can achieve preferential alignment of 1D and 2D carbon nanoparticles, respectively. The first example will be the use of 1D carbon nanofibers in the 3D printing technique. Our approach will be based on the use of stereolithography (SLA) in generating surface patterns and the utilization of layer-by-layer (LBL) assembly to selectively deposit the nanofibers on desirable locations. The drying thermodynamics and the confinement effects from the surface template arranged the nanoparticles with different morphologies and preferentially oriented nanofibers were observed with the control of inter-nanoparticle interactions. The second demonstration involves the alignment of 2D graphene that is challenging to obtain as compared with their allotropes, carbon nanotubes. Free-standing graphene will fold, crumple or wrinkle at ambient temperature due to their instability of thermodynamic states. Our manipulation of nanoparticle-polymer interfacial interactions will first constrain the graphene layers within specific region, followed by the macrolecular movements-generated shear and rotating moments, thus producing aligned graphene layers laminated between polymer channels. These two projects depend on our design and development of in-house manufacturing setups. The processed composite fibers and films were examined with their nanoparticle alignment, the mechanical reinforcement, and the functional properties (i.e., electrical conductivity, sensing of mechanical strains, chemicals, and VOCs). The unique manufacturing and composites have broad applications in wearable, robotics, biomedical, and other areas.

Key Words: Carbon, fiber, 3D printing, sensor

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Abstract ID: 145

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Embedded Nanoparticles and Nanocomposite Films

Keywords: Aluminothermic reduction, Si nanoparticles, Heterojunction thin-film solar cells

Facile Synthesis of Silicon Nanoparticles from the Padma River Sand of Bangladesh and Their Application in Thin-film Solar Cell

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In the quest of a cost-effective and environmentally benign process for the production of Silicon (Si) from the abundant river-sand, this research presents an investigation on a modified aluminothermic process, which is low-cost, low-energy and CO2 free, compared to the conventional carbothermic process for the extraction of Si from sand. Also the efficacy of synthesized Si nanoparticles (Si-NPs) from the produced silicon in photovoltaics has been presented. Si was extracted as eutectic mixture of Aluminium and Si after the aluminothermic process and highly pure (>98%) polycrystalline silicon was obtain with 3-cycles of HCL leaching. Low-temperature mechanical milling was used to make this silicon into powder. After cleaning and drying, Si powder was treated with a solution of hydrofluoric (HF) acid and 2-propanol that provided etching of the native oxide and passivation of the dangling bond with hydrogen (H). Later ultrasonication was performed on the Si powder for crushing them into tiny particles. XRD confirmed the amorphous nature Si particles. Dynamic Light Scattering was used to determine the size distribution profile for three different duration of sonication. Higher sonication time fabricated lower particle size of Si. It was found that the average size of the Si-NPs was controllable and was dependent on the duration and power of the ultrasonication. Si-NPs-doped CuO thin film as absorber in ZnO/CuO based thin-film solar cell was synthesized from cupric acetate using a simple one-pot process and was deposited onto glass substrate using spin-coating. The optical absorption of CuO and hence the conversion efficiency of fabricated solar cell was found to be influenced by the incorporation of Si-NPs in their lattice. Experimental results shows a huge potential for the experimented process and produced silicon to be a game changer for the global energy security, particularly for Bangladesh, where solar energy and river sand are considered abundant and renewable sources.

Abstract ID: 146

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Electro-thermal properties of composite materials

Keywords: Carbon Fiber Composites, Electrical Conductivity, Lightning Strike, Carbon Nanotube

Improved Electrical Conductivity of Carbon Fiber Composites for Lightning Strike Protection through Premixing Epoxy Resin with Carbon Nanotube Particles

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It has been decades since the first application of composite materials in industries. Carbon fiber composites, due to its light weight and high strength, are of especial interest in aerospace industries. Though the reinforcing carbon fiber materials are electrically conductive, the addition of the non-conductive resin matrix makes the overall composite laminates non-conductive which leads to the necessity for additional protection against lightning strikes. Common lightning strike protection (LSP) methods involve stacking an additional layer of copper mesh or extended metal film on top of the composite laminates which results in additional manufacturing costs and special treatment between bonding layers due to the galvanic corrosion. Our previous work was an attempt to offer a potential solution for LSP by adding carbon nanotube (CNT) additives to the resin system to improve the overall electrical conductivity of the composite laminates. In our previous work [1], Adtech 820 epoxy resin with (premixed with CNT by the manufacturer) and without the CNT additives were used to fabricate the carbon fiber composite laminates. Four-point probe tests showed a 31% decrease in electrical resistance for carbon fiber composite laminates. Due to the small test specimen sizes (6×6 inch), the simulated waveform A lightning strike with a peak current of 100 kA yielded no visible damage to our test laminates since the lightning strike was believed to be partially conducted by the grounding fixtures around the test specimens. The current work is a continuation of our previous work where varying weight ratios of CNT will be mixed with our epoxy resin to fabricate the carbon fiber composite laminates. Simulated waveform A lightning strike tests will then be conducted followed by ultrasonic scanning and SEM for damage observation, and four-point flexural test for residual strength.

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Abstract ID: 147

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster/Oral Presentation

Topics: Advances in electrolyte and electrolyte additives

Keywords: Keywords: Ilmanite, Titanium dioxide nanomaterials, Magnetite nanomaterials, Zero-valent iron-Fe2O3 core-shell structures, Electronic nanomaterials, Magnetic nanomaterials

Hydrothermal Breaking Down of Natural Ilmanite into Pure Titanium dioxide and Iron oxide Nanomaterials under Mild Conditions for Low-cost Production of Electronic and Magnetic Materials

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Industrial scale production of electronic nano-materials such as TiO2 and magnetic nano-materials such as magnetite and zero-valent iron starting from impure natural minerals such as ilmenite is of considerable interest for their practical utilization. Current methods for converting ilmenite to titanium dioxide products are based on chloride and sulphate processes which demand drastic conditions and use of hazardous chemicals thus imposing adverse effects on the environment. Herein we report a novel method based on hydrothermal treatment followed by refluxing/coprecipitation at 170 ºC as opposed to 1200-1400 ºC required for current processes. Here the hydrothermal breaking down of ilmenite to titanium oxychloride and iron chlorides is achieved using minimal amount of 9 M HCl by filling 70% volume of the revolving autoclave closed system and subjecting to hydrothermal treatment, at 170 ºC, for 4 h where titanium component together with silica impurities are separated as a solid precipitate and chlorides of iron(II) and iron(III) go in to the supernatant. The slid precipitate is subjected to reflux under basic conditions with a few drops of hydrogen peroxide for 1 h where Na2Ti3O7 is dissolved separating silica impurities as the solid precipitate. The supernatant containing Na2Ti3O7 is again treated hydrothermally with hexadecyltrimethylammonium bromide (HDTMA) at its critical micelle concentration at 100 ºC for 1 h. The crude product Na2Ti3O7 is sonicated with minimal amount of acetic acid for the exchange of Na+ for H+ present in the interlayer spaces of Na2Ti3O7. The calcination of Na2Ti3O7 at different temperatures in the range from 300 ºC to 800 ºC gives TiO2 nanomaterials with well-controlled morphologies in different crystallographic phases from nanoflows, nanorods and nanowires. The initial supernatant containing iron chlorides is converted to 1:3 molar ratio of Fe(II):Fe(III) using required amount of KI and magnetite nanoparticles are precipitated at pH 9-11range using a base such as NaOH or NH4OH and sonicated in water. Zerovalent iron nanoparticles encapsulated in Fe2O3 shell are prepared by the green synthesis using polyphenols present in tea extract in nitrogen atmosphere. Materials synthesized are well characterized using XRD, SEM-EDAX, FT-IR and BET surface area measurements.

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Abstract ID: 148

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Solar Cells

Keywords: diamond-like phases, heat capacities, similarity method, Debye's functions, thermodynamics

Analysis of the Thermodynamic Properties of Functional Materials with a Diamond-like Structure

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Analysis of the Thermodynamic Properties of Functional Materials with a Diamond-like Structure

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The primary goal of this work is the standardization of physicochemical constants.

Previous review articles [1, 2] established a strict relationship between the enthalpy of formation, melting point and the atomic numbers of components in the semiconductor AIIIBV phases, with the diamond-like structure of sphalerite and wurtzite types. The proposed model was used for the critical assessment of the thermodynamic properties of isostructural compounds. The relationship between the reduced enthalpy, standard entropy, reduced Gibbs energy and the sum of the atomic numbers (Zi =ZA+ZB) has been used for a critical assessment of the thermodynamic properties of AIIIBV phases.

The similarity method was applied for the critical analysis of specific heats Cp (T) for solid state of the AIIIBV isostructural phases. A critical analysis of heat capacities was carried out for the pure elements of the Periodic System fourth group (C, Si, Ge, Sn) and isostructural phases AIIIBV and AIIBVI. It was found that the dependence of the heat capacities Cp (T) from 0 to 1500 K follows certain regularity.

Phases with the same sum of the atomic numbers of elements (Zi), such as BN (hex) Zi = 12 and glassy pure carbon Z = 6; BP and AlN (Zi = 20); AlP (Zi = 28) and pure Si (Z = 14); BAs and GaN (Zi = 38); AlAs and ZnS (Zi = 46); AlSb, GaAs, InP (Zi = 64) and pure Ge (Z = 32); GaSb, InAs, and CdSe (Zi = 82); InSb, CdTe (Zi =100) and pure grey Sn (Z= 50); have the same heat capacity experimental values of the solid state within the experimental uncertainty. This rule can be applied to different isostructural compounds.

The continuum of Cp (T) vs. logarithm of the sum of atomic numbers of elements of the AIIIBV phases (sphalerite and wurtzite types) allowed to evaluate the Cp (T) values of the chalcogenides of mercury, AlP, and TlN at the large interval temperature.

The approximation of the heat capacities of the AIIIBV, AIIBVI phases and pure elements of the fourth group (C, Si, Ge, Sn) was accomplished by a linear combination of Debye's functions [3].

The similarity method is convenient for the critical analyses of the heat capacities and can be applied to not only the diamond-like isostructural chemical compounds (binary, ternary and multi-component systems) but can also be extended to other different isostructural substances.

Key Words: diamond-like phases, heat capacities, similarity method, Debye's functions, thermodynamics

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[3] V.P. Vassiliev, V.A. Lysenko, IUPAC and Chemistry, CL367BIS, Paris, France, July 7-12, 2019.

Abstract ID: 149

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Solar Cells

Keywords: Periodic Law, "tetrad-effect" phenomenon, lanthanides, actinides, physicochemical properties

"Tetrad-Effect" Phenomenon for the Lanthanide Compounds and the Pure Actinides

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"Tetrad-Effect" Phenomenon for the Lanthanide Compounds and the Pure Actinides

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Different relationships between the various physical and chemical properties of isostructural compounds take place according to the Periodic Law that is a fundamental basis of Chemistry.

The "tetrad-effect" phenomenon was established and used for the analysis, correction and prediction of thermodynamic data for the lanthanide (Ln) compounds and the pure actinides (Ac). They are connected to the 4f-electrons of the lanthanide elements (Ln: La-Lu; their atomic numbers are 57-71) and 5f-electrons of the actinides with atomic numbers from 89 to 102. The most sensitive to the tetrad-effect the thermodynamic functions of lanthanide and actinide compounds are standard entropies and entropies of formation, because they are the most susceptible to the influence of the 4f- and 5f electrons of the lanthanides and the actinides. We analyzed some classes of lanthanides with other elements of the Periodic Table, which account for only a sampling of the thousands of similar binary compounds possible. As an example, we use the tetrad-effect concept for the analysis and prediction of the standard entropies of the solid phases as the Ln2X3 (X=O, S, Se, Te). This approach can also be applicable to other classes of the Ln compounds as LnN, LnB2, LnB4, LnB6, LnF3, LnIn3 and other compounds. Unfortunately, the actinides and the alloys on the base these elements are studied insufficiently, but it is possible to apply to them the same laws.

Key Words: Periodic Law, "tetrad-effect" phenomenon, lanthanides, actinides, physicochemical properties

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July 7-12, 2019.

Abstract ID: 150

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: All solid-state batteries

Keywords: Tape-casting, all-solid-state battery, energy storage

Design-of-Experiment (DoE) Guided Optimization of Slurry-Coated Cathodes for All-Solid-State-Batteries

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All-solid-state batteries (SSBs) are being considered as viable energy storage technology, possibly possessing higher energy and power densities (and improved safety) than conventional lithium-ion batteries (LIBs) [1]. Laboratory research into bulk-type SSBs has been focused predominantly on pelletized cells, sufficient to evaluate fundamental limitations and to optimize the constituents to some extent. However, a slurry-based fabrication process for SSBs showing little to no performance loss, as compared to the pelletized counterpart, is required, especially regarding the commercial implementation of such technology. In order to speed up the development of such process, we have used a design-of-experiment (DoE) guided approach to evaluate the influence of different parameters (i.e., type of binder, solvent, carbon additive) on the electrochemical performance of tape-cast cathodes in SSB cells. Although such SSB cathodes approach the performance of their conventional fabricated LIB cathodes, they still deliver lower specific capacities and show some fading. In order to shed light on the origin of such limitations, we monitored structural changes and gas evolution of the cathode layer by means of operando synchrotron X-ray diffraction (XRD) and differential electrochemical mass spectrometry (DEMS), respectively [2,3].

Key Words: tape-casting, all-solid-state battery, energy storage

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Abstract ID: 151

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: ey Words; Binary separations, Cellulose acetate, Characterization, Nanocomposite, Sol-gel method.

Synthesis and Characterization of Cellulose acetate titanium (IV) tungstomolybdate Nanocomposite Cation Exchanger for the Removal of Selected Heavy Metals from Aqueous Solution

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ABSTRACT: novel Cellulose acetate titanium (IV) tungstomolybdate nanocomposite cation exchanger was synthesized by sol-gel method by incorporating cellulose acetate polymer into inorganic exchanger, titanium (IV) tungstomolybdate. Different techniques including FTIR, XRD, TGA SEM and BET were used to characterize the exchanger. The Cellulose acetate titanium (IV) tungstomolybdate (CATTM) behaved as a good cation exchanger with IEC of 1.64 meq g-1 for Na+ ions. The sequence of ion exchange capacity for alkali metal ions was found to be K+> Na+> Li+ and that for alkaline earth metal ions was Ba2+ > Ca2+ >Mg2. These orders revealed that the ions with smaller hydrated radii acquired larger ion exchange capacity. The pH titration curve indicated that the material obtained as such is a bi functional strong cation exchanger as indicated by a low pH (~2.25) of the solution when no OH- ion was added. Thermal analysis of the material showed that the material retained 50% of its ion exchange capacity up to 600°C. Adsorption behavior of metal ions in different solvents with varying concentration has also been explored and the sorption studies revealed that the material was selective for Cr(III) and Pb(II) ions. The analytical utility of the material was investigated by performing binary separations of selected metal ions in a column based on the distribution coefficients of the metals. Cr(III) and Pb(II) were selectively removed from synthetic mixtures of Cr(III)-Cd(II), Cr(III)-Fe(III), Pb(II)-Cd(II) and Pb(II)-Fe(III). Antimicrobial activity of the synthesized inorganic compound was evaluated and showed a considerable antibacterial activity against Staphylococcus aureus, Streptococcus agalactiae, Escherichia coli and Shigella flexneri. The inorganic counterpart has also exhibited a promising antifungal activity against Aspagilus niger and Fusarium oxysporim.

Abstract ID: 152

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Sandwich materials/hybrids, Multifunctional composite, Advanced composites

Keywords: DNA, synthetic biology, bio foam, biomaterial, biodegradable

GMO Biodegradable Biofoam Material

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GMO BIODEGRADABLE BIOFOAM MATERIAL

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Natural biomaterials are usually made from plant and/or animal sources, however they can pose some disadvantages including unpredictable availability due to weather conditions, pests and/or diseases, change of cost, as well as competition from human demands from fibers or food. Therefore, we are the first to produce genetically synthesized biofoam, and this process is carried out by ensambling different natural and synthetic genetic parts including genes and proteins, which are cloned in a known pathogenic yeast or bacteria, towards production of a target protein and/or biomolecule to obtain a biofoam, using the most recent novel approach of synthetic biology , hence, constructing a bio fabric for production of biofoam. The key elements for ensambling this gene towards the production of the biofoam are the selection of the natural source of genes, the types of genes, the types of vectors, and the type of microorganism which host the construct DNA or genetic ingredients for production of the biofoam. Our genetic approach allows us to tailor biofoams with different polymeric size, texture (i.e. hardness, and/or memory), for different applications including industry, agriculture, and suitable for environmental protection. Also, another important aspect for production of our bio foam is the fermentation process which guarantee not only good growth of the microorganism, but also yield and production of the biomaterial which will constitute the ingredients for the biofoam. Furthermore, our GMO biomaterial, such as bio foam could be made with inherent antimicrobial ingredients. We were able to make biofoams of different sizes, textures, and for different applications, including cups for beverages, pots for agricultural use, laminar material for book or paper protection, as well as materials for seats use of automobile/aircrafts, office and home. Also, our genetic biofoam can be used as an insulating material, and for stimulating plant germination.

Abstract ID: 153

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Resources for battery materials

Keywords: Synthetic biology, Nutritionally Modified Organism, Microbial electrical circuit, light, biomechanical movement.

GENETICALLY OR NUTRITIONALLY MODIFIED ORGANISMS FOR THE PRODUCTION OF LIGHT OR MECHANICAL ENERGY: A HEATLESS ELECTRIC MICROBIAL CIRCUIT (HEMC)

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GENETICALLY OR NUTRITIONALLY MODIFIED ORGANISMS FOR THE PRODUCTION OF LIGHT OR MECHANICAL ENERGY: A HEATLESS ELECTRIC MICROBIAL CIRCUIT (HEMC)

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Patent Pending

Here we describe a unique source of light produced by extracts derived from a nutritionally modified organism (NMO) or from a genetically modified organism (GMO). The phenotypic or genotypic characteristics of the microorganisms produce light and mechanical energy (e.g., power the movement of small motor gadget). Redox, pH, and growth of the microbial culture were correlated to the results. Extracts of the NMO or GMO culture were used as a liquid or slurry at different concentrations as a light source in a light emitting diode (LED). Different wavelength LEDs were used to express the photonicity of the heatless electrical microbial circuit or mechanical energy. This microbial circuit was connected through electrodes to the microbial extract contained in different tubes in a serial display, where the other end of the circuit was connected to different LEDs or a small, vibrating cellular phone. The efficacy of this HEMC was based on, voltage, amperes, watts, current, duration of photoluminescence, and intensity. The results showed significant voltage (e.g., > 4 volts) and current to produce intense light at different LED colors for extended periods of time. The microbial extracts can also be used to stimulate growth of both plants and yeast. This investigation not only unlocks the secrets of nature, but also benefits society by providing cost-effective light, particularly to countries that cannot afford electricity, while protecting the environment. The microbial extract with biophotonic characteristics can be applied to different industrial processes, and as a source of renewable energy to power mechanical and electronic devices.

Abstract ID: 154

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Anodes and cathodes Materials

Keywords: Ferrates, Fuel Cell Cathodes, Phase Diagrams, SOFC, Ab Initio Thermodynamics

Thermodynamic stability of La, Bi, and Sr ferrates : a hybrid DFT study

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Ferrates of Bi, La, and Sr are the end members of wide set of solid solutions (Bi1-xSrxFeO3-δ , Bi1-xSrxFe1-yCoyO3-δ, and La1-xSrxFe1-yCoyO3-δ). These materials are mixed ionic-electronic conductors and, therefore, have potential to be used or are already used for intermediate temperature cathodes of oxide fuel cells and related electrochemical and catalytic devices. In addition, BiFeO3 perovskite attracts great attention due to its multiferroic properties. Also, SrFeO3-δ has complex magnetic structure revealing colossal magnetoresistance effect what makes it interesting for spintronic applications; its properties strongly depend on oxygen non-stoichiometry. In this study ab initio hybrid functional approach was used for a study of thermodynamic stability of the considered ferrates with respect to their decompositions into binary oxides and to elements, as the function of temperature and oxygen pressure. The atomic (LCAO) basis sets were carefully re-optimized within the CRYSTAL computer code. Based on our calculations, the phase diagrams were constructed allowing us to predict the stability regions of BiFeO3, LaFeO3 and SrFeO3-δ (δ=0, 0.125, 0.25, 0.5) in terms of atomic chemical potentials. This permits determining environmental conditions for existence of stable phases with the above-mentioned compositions. These conditions were presented as contour maps of oxygen atom chemical potential as a function of temperature and partial pressure of O2 gas. A similar analysis was also performed using the experimental Gibbs energies of formation. The present modelling of SrFeO3-δ strongly suggests a considerable attraction between oxygen vacancies. These vacancies are created during a series of above mentioned SrFeO3-δ mutual transformations (δ=0→0.125→0.25→0.5) accompanied by oxygen release. It is shown that (within employed model) only the SrFeO2.5 phase appears to be stable in O2 -gas atmosphere.

Key Words: Ferrates, Fuel Cell Cathodes, Phase Diagrams, SOFC, Ab Initio Thermodynamics

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Abstract ID: 155

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Bio-composites

Keywords: Bioactive Hybrid Gelatine Microgels; Bacteriophages; Mesenchymal Stem Cells

Multifunctional Bioactive Hybrid Gelatine Microgels Carrying Bacteriophages and Aggregates of Mesenchymal Stem Cells

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This study attempts to prepare bioactive hybrid materials for treatment of mainly chronic wound infections like “Diabetic Foot Infection” - “DFI”) and “Diabetic Foot Osteomyelitis - “DFO”) using a combinational therapy. As bioactive materials bacteriophages as antibacterial agents and mesenchymal stem cells (MSCs) for regeneration of both soft and hard tissue were included within the formulations. Gelatine microgels around 50-100 micron were selected as the carrier matrices. Both native/plain gelatine and its cationized forms were used as alternatives to prepare microgels. Cationization was achieved by amination of gelatine chains using ethylene diamine by carbodiimide chemistry. The extent of the amino groups introduced was about 21%. Gelatine microgels were then prepared by dispersing both the plain and cationized gelatine within an oil phase to obtain water-in-oil dispersions, the resulting spherical gels were cross-linked dehydrothermally and dried. In order to increase stability and their availability in longer periods in the wound area bacteriophages were loaded/immobilized in/on gelatine micogels by simple sucking technique. As a model target E.coli and its specific bacteriophages were propagated in standard bacterial cultures. Bacteriophages were labelled by FTIC for imaging of both loading and release on/from the gelatine microgels. Microgels with different size, cross-linking densities made of different materials (i.e., plain and cationized gelatine) carrying different amounts of bacteriophages were compared by following loading efficiencies and activities of the immobilized bacteriophage formulations on the target bacteria. MSCs were isolated from the adipose tissue from mice, cultured and aggregates were formed with or without the microgels carrying bacteriophages. The aggregate forms/sizes, cell densities and viabilities were followed in two week’s 3D cultures and compared focusing on the microgel formulations.

Acknowledgement: E. Piskin has been supported by the Turkish Academy of Sciences as an honorary member.

Abstract ID: 156

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Computational Electronic Materials

Keywords: Co based Heusler, First principle study, DFT, Structural, Electronic Property.

An Ab Inito study of Structural, Electronic, Mechanical and Vibrational Properties of VCo2Al

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The class of Semimetals has emerged as upcoming future devices due to their technological efficient applications. The distinguishing feature in Semimetals is the simultaneous manipulation of spin states along with electronic states that has led to the discovery of spin ordering at Fermi level. The present study is first principle approach to compute structural, electronic, mechanical and vibrational properties of VCo2Al. The theoretical investigation will be made based on Density Functional Theory (DFT) and Density Functional Perturbation Theory (DFPT). The predictions of physical properties from these calculations would create future scope of experimental work for further realization of fascinating applications of VCo2Al.

Abstract ID: 157

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Dielectric materials

Keywords: Porcelain, Alumina, Permittivity

Dielectric Algerian Triaxial Porcelain With Al2O3 and Al(OH)3 as Additions

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Porcelains represent the foundation of the ceramic discipline. The production of porcelain, for the ceramic dielectric applications by using inexpensive natural raw materials or waste materials was undertaken. The principal raw materials of porcelain, such as kaolin, feldspar, and quartz, are relatively inexpensive and readily available. The raw materials used in this study were collected from Algerian source (Kaolin was from Debagh deposit, Quartz from El Oued city and Feldspar from Ain Barbar deposit). In an earlier study, a basic electro-porcelain composition was selected consisting of 37% kaolin, 35% potash-feldspar and 28% quartz. The dielectric properties of porcelain bodies prepared without the incorporation of mineralisers or metal oxides, e.g. dielectric constant, dielectric loss tangent (tan δ) and factor loss, were investigated. Dielectric measurements have been carried out at 1 kHz in the temperature range ambient Temperature – 200°C. The dielectric constant ε' and dielectric loss tangent tan δ respectively of porcelain samples sintered at the most proper sintering temperature 1200°C were about 21.22 and 0.006. The value of dielectric constant is higher as compared to conventional porcelain which not exceeds generally 9. In this study, the dielectric of porcelains containing Al2O3 and Al(OH)3 was investigated. Al2O3 and Al(OH)3 were added in the initial mixture. The dielectric characterization of fired porcelain, at 1100°C, shows that permittivity value can be increased depending in Al2O3 and Al(OH)3 content.

Abstract ID: 158

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: Key Words: Nanomaterials, Biosensors, Cytokines, Surface modification, Medical devices

Engineering nanomaterials based multi-functional interfaces for cytokine biosensing: from nanosensors to in vivo medical devices

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Cytokines, low molecular weight (~6-70 kDa) soluble proteins secreted from the immune and non-immune cells are core indicators of the functional status of the body. Consequently, monitoring cytokine secretions has enormous value in biology and medicine. Unfortunately, probing cell secretions as they respond in real time to the surrounding signals is still a major challenge as the processes tend to be transient and small molecular size of cytokines, combined with low concentration (in the pM range) and possible interferences in matrix samples. The traditional method for cytokine detection relies on ELISA, which however is expensive, time consuming and incapable to realize real-time monitoring.

By integrating with nanotechnology, biosensors as the analytical devices for the detection of an analyte, that combines a biological component with a physicochemical detector, have demonstrated huge potential for cytokine sensing. Functional nanomaterials possess good conductivity, catalytic activity, biocompatibility and high surface area. This presentation will highlight our recent studies on engineering the sensing interface with functional nanomaterials to achieve novel biosensors for detection of cytokines with improved performances in terms of sensitivity, selectivity, stability and simplicity. These nanomaterials powered sensing platforms include nanosandwich assays, nanosensors, and graphene oxides based andaptasensors, which can be applied for cytokine detection from point-of-care diagnostics to in vivo real-time monitoring. The strategies for fabrication of non-fouling biosensing interface will be discussed. Finally, strategies for fabrication of hydrogel based biosensing devices such as sweat wearables and implantable chips, for continuous cytokine monitoring, will be presented.

Key Words: Nanomaterials, Biosensors, Cytokines, Surface modification, Medical devices

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Abstract ID: 159

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: TiO2; EG; Photocatalysis; Self-cleaning

Fabrication of ultrafine nano crystalline anatase TiO2 with enhanced functional properties

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Anatase form of ultrafine TiO2 with higher crystallinity was synthesized by sonication. The growth of the nano crystals was suppressed by using ethylene glycol during the reaction mechanism. Central composite design was used to investigate the effects of process variables. The as-synthesized nanoparticles were characterized by SEM (scanning electron microscopy) and XRD (X-ray diffractometry). Functional properties i.e. photocatalytic performance, ultraviolet protection factor, self-cleaning efficiency have also been investigated. Photocatalytic performance was investigated against MB (methylene blue) which is considered as model organic pollutant in many industries. A comparison was made with commercially available photocatalyst P25 for better photocatalytic performance. Maximum 99 % dye was removed by as-synthesized TiO2 under optimal conditions. Interestingly, functional properties were not changed after calcination.

Abstract ID: 160

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Durability and Ageing of Composite Materials and Structures

Keywords: mathematical modeling, OSB composite, mechanical properties, weathering

Prediction of Modulus of Rupture Decay of OSB Composite exposed to natural weathering by means of Artificial Neural Networks (ANN)

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The present study aimed to predict the modulus of rupture (MOR) decay of Oriented Strand Board (OSB) composites, exposed to natural weathering, using Artificial Neural Networks (ANN), a modern and powerful data processing tool which is able to solve complex problems. Periodic evaluations were performed at 0, 3, 6, 9 and 12 months of exposure to natural weathering, to collect the specific mass (ρ) and the mechanical properties of dynamic modulus of elasticity (Ed) and modulus of rupture (MOR). These factors (ρ, Ed, and time of exposure) were used as estimators of modulus of rupture by the application of Multilayer Perceptron networks, training 1000 of them for each of the evaluated parameters. Also, Multiple linear regresion (MLR) was run and compared with ANN approach. The selected network presented a 3-10-1 topology, a correlation (r) of 0.98 and a standard estimated error (Syx%) of 6.83%. The validation process showed no statistical difference between observed and predicted values. On the other hand, r and Syx% values for MLR were 0.70 and 20.57%, respectively, and validation showed values statistically different. The obtained results indicated that the use of Artificial Neural Networks is an efficient tool for predicting the decay of OSB composite resistance.

Abstract ID: 161

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Nanocomposites

Keywords: Metal Insulator nanocomposites, CNT based nanocomposites, Field emission device, First principle based calculation

Metal nanoparticle embedded in insulating matrix and nanoparticle decorated MWCNT: a new generation field emission source based devices

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We present here magnetic and field emission (FE) properties of two types of nanostructured composite films, promising novel materials for third generation electron sources and displays: (i) Nanoparticle decorated multi-walled carbon nanotubes (MWCNTs)-and (ii) metal-insulator nanocomposite thin-films. FE measurements were carried out in an indigenously developed high vacuum diode set up. The salient results obtained can be summarized as (i) a significant improvement of FE current and temporal stability associated with an appreciable reduction in turn-on field from metal nanoparticle decorated MWCNT-films as compared to only MWCNT films: showing promises for electron-guns, x-ray sources etc.; (ii) appreciable increase in FE current density with high mechanical durability in metal nanoparticle decorated composites: promising planar emitter for future flat-displays. The enhanced FE characteristics of these emitters are understood from a combined experimental results, electronic structure first-principles based calculations study. Magnetic anisotropy effect has been demonstrated for the magnetic nanocomposite films.

Abstract ID: 162

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: Ferroelectrics, PLD, Rare-earth, Energy storage.

Recoverable Energy Storage Properties on Pb-based and Pb-free Ferroelectric Thin Films

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Pb(ZrxTi1−x)O3 (PZT) has been widely used for energy storage applications because of its excellent ferroelectric and piezoelectric properties compared to other ferroelectric materials. The present study describes the influence of rare-earth (RE = La, Eu, Dy and Ho) ions on recoverable energy storage density in PLD grown epitaxial PZT thin films on SRO/LSAT (001) heterostructures. The enhancement of spontaneous polarization in the donor (La, Eu) doped PZT films compared to the pure one is attributed to easy orientation and mobility of domain walls. It is found that the piezoelectric coefficient (d33) is more (130 pm/V) for La doped PZT films (La:PZT), compared to the other rare earth doped PZT thin films. In our results, we found asymmetric polarization versus electric field hysteresis loop and energy storage efficiency (η) values of 30% were recorded in the case of pure PZT film and the value decreased to 28% with Ho doping5. However, a high value of 46% could be realized in La:PZT as shown in figure 1. The results will be presented and discussed in details.

Abstract ID: 163

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Optical properties of metals and non-metals

Keywords: WGM, micro sphere, RE doping, lasing

WGM lasing from Sm 3+ ZnO micro spheres fabricated by laser ablation technique

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Whispering gallery modes (WGMs) from dielectric micro cavities possess very small mode vol ume and high quality (Q) factor, are f ind applications in nonlinear optics, micro lasers, ultra sensitive molecular sensors , etc Being a wide bandgap material (Eg = 3.37 eV), ZnO is one of the suitable hosts for rare earth (RE) ions [To realize RE specific 4f emissions in the visible spectral range, interband levels are c r eated in the bandgap of ZnO by doping with suitable RE ion s [2]. In the present study h ighly smooth and crystalline Sm 3+:ZnO microspheres were synthesized by laser ablation process using sintered target s in air. Sharp WGM resonances in the visible range ~ 550 750 nm are observed due to the coupling of Sm 3+ f f transitions namely, 4 G 5/2 □ 6 H J (J=5/2, 7/2, 9/2 and 11/ to the WGMs of the Sm 3+:ZnO microcavity . The resonances are found to be lasing above low threshold and have Q factor of the order of 10 3 . These results could be useful for light emission and sensing applications which operate in the visible spectral range.

Abstract ID: 164

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Point Defects, Doping and Extended Defects

Keywords: Doping, conductivity, implantation.

Observation of enhanced conductivity in n type nano crystalline diamond implanted with nitrogen and phosphorus

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Diamond is known as an ‘ultimate engineering material’ because it possesses extreme properties suitable for various applications including highest thermal conductivity, high hardness, transparent over a wide range of frequencies, highly incompressible, and highly resistant to chemical reactions. Doping of diamond further multiplies its area of research, for example, through nitrogen doping and boron doping, the bandgap of diamond can be engineered. Resistivity and grain size of diamond films can be tuned to suit various applications in the field of electronic devices. Quantum qubits can be generated in diamond where quantum information processing can be efficiently realized. However, Diamond (bandgap, Eg = 5.47 eV) suffers from an asymmetric doping problem and thus, n type doping is relatively difficult compared to p type. Introduction of boron atoms into the sp3 bonded carbon network of diamond creates impurity levels at 0.36 eV above the valence band maximum (VBM). When heavily doped with boron, the impurity levels aggregate into a band. Beyond a critical concentration for the insulator to metal transition (IMT), impurity band merges with the valence band. Therefore, at high boron concentration (~ 4.5 x 1020 cm 3) diamond becomes a superconductor1,2,3,4. This has been well studied by many groups. Our group is currently working on realizing n type diamond by ion implantation with nitrogen and phosphorus which are the potential n type donors. Doping nitrogen to a level to induce insulator to metal transition has been a big challenge which we have succeeded and we have observed that doping with nitrogen and phosphorus in ultra nanocrystalline, nanocrystalline and even single crystal diamond has brought enhanced conductivity along with insulator to metal transition which was clearly evident in transport properties. The development of high quality n type diamond thin films with such high conductivities has potential applications in diamond based electronic devices and quantum computing.

Abstract ID: 165

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Industrial applications of composite materials

Keywords: Textile, Adsorption, Noble Metals, Ammonia

Adsorption, Enrichment and Recovery of Resources and Pollutants by the Use of Functional Polyelectrolyte/Fiber Composites

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The recycling and recovery of high-prized noble metals such as platinum, gold, palladium and silver or rare and strategic metals like indium, gallium, and rare earth metals from scrap metals and wastewaters will be from steadily increasing importance within the next years. Therefore, the focus has to be set on the detection of potentially usable secondary resources and the development of inexpensive and energy-saving processes to separate and recover the metals selectively (urban mining). Beside electronic scrap industrial process and wastewaters represent a considerable source for noble metals. Recently, we have successfully developed an innovative metal-adsorbing textile filter material based on various polyelectrolytes. The surface modification of the fibrous material is easy to realize with common methods in textile finishing yielding a durable, high-performing and even cheap fiber-fixed polymer network. We present results on the general textile finishing procedure and the pH-depending adsorption of noble metal ions. The feasibility of the overall process is demonstrated on various palladium containing process waters obtained from producers of curcuit boards and metal plating industry. Moreover, the same innovative adsorber material is useful for the decontamination of, e.g., chromate-polluted ground waters and soils. Our latest investigations focus their use in the adsorption from gaseous phase - namely the adsorption of ammonia. Ammonia has a negative impact on the environment and health. It causes particulate matter pollution and plays an important role in global warming because it can be transformed to climate-damaging nitrous oxide. The most important pollution emitter is the farming industry. Here, we present our first promising results on the direct adsorption of ammonia in pigsties and the transformation into valuable mineral fertilizers.

Abstract ID: 166

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Novel Magnetic Materials and Device Applications

Keywords: Chiral induced spin selectivity, spintronics devices, chiral separation, exchange interactions

Chirality and the Electron Spins

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With the increasing demand for miniaturization, nano-structures are likely to become the primary components of future integrated circuits.Different approaches are being pursued towards achieving efficient electronics, among which are spin electronics devices (spintronics) [1]. In principle, the application of spintronics should result in reducing the power consumption of electronic devices.

A new, promising, effective approach for spintronics has emerged using spin selectivity in electron transport through chiral molecules, termed Chiral-Induced Spin Selectivity (CISS) [2]. Recently, by utilizing this effect we demonstrated a magnet-less magnetic memory [3,4]. Also we achieve local spin-based magnetization generated optically at ambient temperatures [5,6]. The locality is realized by selective adsorption of the organic molecules and the nano particles [7]. Lastly we have been able to show chiral proximity induced magnetization on the surface of ferromagnetic and superconducting materials. The magnetization is generated without driving current or optically exciting the system [8,9]. Interestingly, the opposite effect supplies a simple new spin interaction which enables enantio-selection. The interaction of chiral molecules with a perpendicularly magnetized magnetic substrate is enantio-specific [10]. In the talk I will give a short introduction about spintronics and the CISS effect. Then I will present ways to achieve simple spintronics devices utilizing the effect.

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Abstract ID: 167

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Polymeric composites

Keywords: Polymer Bionanocomposites, Fire retardancy, Gas-barrier properties

Designing Clay Modified Polysaccharide-Based Bionanocomposite: An Emerging Eco-friendly Fire Retardant Material

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Despite abundant researches on petroleum-based polymer nanocomposites over micro and macro composites, these nanocomposites suffer from deprived biodegradability, highly inherent flammability and less mechanical strength. Novel multicomponent polysaccharide based bionanocomposites such as (Cellulose-g-polybutyl acrylate) / kaolin, (carboxymethyl cellulose-g-polyacrylonitrile) / montmorillonite, (guar gum-g-polybutyl acrylate) / montmorillonite were synthesised via graft copolymerization of acrylate-based monomer onto polysaccharide and incorporation of nanoclay by using APS as a free radical initiator, in the presence of MBA as a crosslinking agent to design materials with negligible or no environmental hazards. Among the above bionanocomposites, the morphology of (GG-g-PBA)/MMT was confirmed by FTIR. The XRD and TEM observations revealed that MMT was exfoliated and uniformly dispersed in GG-g-PBA matrix. The resultant bionanocomposite showed remarkably improved thermal stability and mechanical properties. In addition, the excellent fire retardancy of the bionanocomposite results from the formation of compact and continuous char which not only hinders the migration of volatile decomposition products out of polymer matrix but also provides barrier for heat transfer evaluated by limiting LOI and cone calorimeter test. The biodegradation test has been carried out for better commercialization and environmental concern.

Abstract ID: 168

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Electrical, optical, electrochemical, thermal and mechanical properties of graphene, Mxenes and other two-dimensional materials

Keywords: Recrystallization, Shape memory alloy, Severe plastic deformation, Martensite start temperature.

Effect of Sn on microstructure and mechanical properties of CuZnAl shape memory alloy via severe plastic deformation

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Characterization and mechanical behavior was investigated on Cu-Zn-Al-Sn shape memory alloy subjected to severe plastic deformation by equal channel angular pressing (ECAP). The results of Scanning Electron Microscopy (SEM) and X-ray diffraction (XRD) showed the recrystallization of new α phase in matrix of β phase which plays a vital role in microstructure and martensite start temperature (Ms) and the mean diameter of the grain size was reduced to ultrafine scale. The phase transformation temperatures were studied by differential scanning calorimetry (DSC) which determined that martensite start temperature was reduced after ECAP process, while The result was opposite for CuZnAl. This is the most important effect of Sn on CuZnAl SMA properties. The alloy's Vickers hardness increased rapidly from 180 to 198 through the first pass, and then it increased slowly. The yield and compressive strength of specimens increased after ECAP process.

Abstract ID: 169
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Green Composites
Keywords: biocomposites, biodegradation, polyhydroxybutyrate-co-hydroxyvalerate (PHBV), composting, vermicomposting, freshwater biotope

Biodegradation of PHBV Ternary Biocomposites in Different Environments

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The influence of different environments on biodegradation of polyhydroxybutyrate-co-hydroxyvalerate (PHBV) containing nautral-based plasticizer acetyl tributyl citrate (ATBC), calcium carbonate (CaCO3) and lignin coated cellulose nanocrystals (L-CNC) was studied. A twin-screw extruder equipped with a flat film die (0.4 mm gap size) was used for processing of ternary biocomposites and control samples. Vermicomposting, controlled laboratory thermophilic composting and freshwater biotope were used for evaluation of biodegradation. The influence of characteristics such as pH, temperature, moisture content and flow of oxygen on biodegradation rate was studied. The results of biodegradation showed an intensive degradation rate of ternary biocomposites. The addition 10 wt. % of CaCO3 into plasticized PHBV matrix ensured 56% biodegradation after one month exposition to controlled thermophilic composting, 39% biodegradation in environment of vermicompost and 22% biodegradation in freshwater biotope. Similar characteristic but slightly slower biodegradation rates were observed for ternary PHBV biocomposites containing L-CNC (1 wt. %). In contrast, neat PHBV achieved at the same condition in thermophilic controlled composting 32% biodegradation, only 10% biodegradation in freshwater biotope and 14% weight reduction in vermicompost environment. The results showed that the highest influence on biodegradation rate of neat PHBV as well as PHBV ternary biocomposites has a temperature.

Abstract ID: 170

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanomaterials and Nanotechnology

Keywords: ZnAl2O4:Cr3+, Nano particles, Citric acid, Sol-gel

Effect of Al molar ratio on structural and optical properties of ZnAl2O4:Cr3+ (1.0mol %) nano particles synthesized via sol gel method

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ZnAl2O4 is wide band gap semiconductor with an energy gap of 3.8 eV in which Zn and Al cations are located at the tetrahedral and octahedral site of the cubic structure respectively. It is usually used as a host material for optical activators like rare earth ions or transition metal ion [1, 2]. ZnAl2O4: Cr3+ (1.0 mole %) with zinc to aluminum molar ratio of 1: 1.2 , 1: 1.5 , 1: 1.8 , 1: 2.0 and 1: 2.2 NPs were synthesized by sol-gel technique. Single phase ZnAl2O4: Cr3+ (1.0mol %) with Zn: Al molar ratio of 1: 1.2, 1: 1.5, 1: 18, 1: 2.0 and 1: 2.2 successfully obtained through sol gel technique. The XRD result confirmed the formation of cubic spinel structure with crystallite size increased from 12.85nm and 20.81nm with increase in Zn: Al ratio from 1:1.2 to 1: 2.2. SEM spectra show an increase in average crystallite size with increase in Al3+ precursor molar concentration. The EDS spectrum showed the presence of expected elements (Zn, Al, O and Cr). UV-Vis spectroscopy results revealed that the band gap of nanoparticles observed to decrease with increasing Al3+ molar content. Improvement in PL intensity was observed for samples with Zn to Al molar ratio close to the stoichiometric component of ZnAl2O4 in range of 1: 1.8 to 1: 2.2 with maximum intensity at 1: 2.2. When Zn: Al molar ratio is much smaller than the stoichiometric component ZnAl2O4 and the PL intensity show decrement. Choosing an appropriate molar ratio of Al3+ precursor's during synthesis can affect the properties of ZnAl2O4: Cr for desirable application. All the color coordinates located in violet region of the spectrum indication that the material has the potential to be used as violet emitting phosphors.

Abstract ID: 171

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanomaterials and Nanotechnology

Keywords: ZnO, Nano, Sol-gel

Effect of Pb doping on the structural and optical properties ZnO nanoparticles synthesized by sol-gel method

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In recent year, the study of the ZnO hexagonal wurtzite structure has attracted vast attention as a luminescence material owing to its unique structural, optical, thermal, electrical, and luminescence properties which can be exploited to manufacture promising materials devices [1, 2]. Un-doped and Pb-doped ZnO nanoparticles were successfully synthesized in an ethanolic solution by using a sol-gel method. Structural and optical properties of the samples dependence on Pb concentrations were investigated while other parameters were kept constant to ensure reproducibility. It was observed that the structural properties, particle size, band gap, photoluminescence intensity and wavelength of maximum intensity were influenced by the amount of Pb ions present in the precursor. The XRD spectra for ZnO nanoparticles show the entire peaks corresponding to the various planes of wurtzite structure, indicating a monophasic material. The diffraction peaks of doped samples are slightly shifted to higher angles with an increase in the Pb ion concentration, signifying the expansion of the lattice constants and decrease in the band gap of ZnO. All the samples show the absorption in the visible region. The absorbance spectra show that the excitonic absorption peak shifts towards the lower wavelength side with the Pb-doped ZnO nanoparticles. The PL spectra of Pb-doped ZnO consist of UV emission at 340 nm and two broad visible emissions at 370 and 460 nm with varying relative peak intensities. The amount of Pb concentrations red shifts the 460 nm emission but other emissions are hardly affected. The doping of ZnO with Pb amount up 2 mol% enhances significantly the defects emission but quenches thereafter while UV luminescence is hardly affected. The SEM images also clearly show the change in shape and size of ZnO nano particles with increase in Pb concentrations.

Abstract ID: 172

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Sandwich materials/hybrids, Multifunctional composite, Advanced composites

Keywords: Bimodular Beam, Flexural Vibrations, Effective Laminate

Nonlinear Flexural Oscillations of bimodular beam structures

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The paper is concerned with the modeling and numerical solution of the dynamic response of structures consisting of Bernoulli-Euler beams rigid in shear due to time-variant excitation. The beams are assumed to be homogeneous and show classical boundary conditions. However, they are composed of a bimodular material, thus behaving differently in tension and compression.

Generally, bimodular beams can be modeled as effective two-layer laminates. However, their neutral axis depends on the curvature's sign. Thus, the equations of motion for flexural oscillations are developed by defining an effective composite layered structure with discontinuous natural beam axis. The position of the natural axis follows from a (highly) nonlinear equation that is dependent on both the geometry of the cross-section and the elastic material properties. After an appropriate transformation all calculations are formulated respecting an independent reference axis of the bimodular beam structure.

Within a numerical study structures of various cross-sections are considered showing the influence of the bimodular material on the dynamic response. When considering mode shape expansion, beams can be analyzed numerically by means of a modified Newmark method.

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Abstract ID: 173

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: III-V nanowires, Quantum rods, telecom-band emitters, FEM

Optical properties of strained InAs/InP quantum rod nanowires emitting in the telecom wavelengths

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The emergence of semiconductor nanowires (NWs) as a new class of functional materials has generated a great interest in the scientific community. These NWs show promises in diverse application areas, such as light sources, electronics, photovoltaics and sensor technologies. In this work, we have investigated efficient III-V NWs-based telecom-band emitters grown on silicon substrates. We have grown InAs/InP quantum rod nanowires (QR-NWs) on Si(001) substrates by vapour-liquid-solid (VLS) assisted molecular beam epitaxy (MBE) using gold as catalyst. After the growth, the NWs are 80-100 nm in diameter and 1.5-2 □m in length. These NWs have a wurtzite (Wz) structure with the [0001] axis along the NW growth direction for both InP and InAs materials. Due to the high V/III beam equivalent pressure ratio, no stacking faults or cubic segments were observed in the NWs. Optical studies performed at cryogenic temperature reveal a InAs QR emission in the telecom band with two peaks. Finite element method (FEM) calculations taking into account strain effects around the InAs QR were developed to explain these experimental results. Temperature-dependent optical properties revealed high stability of the PL intensity in the 14–300 K temperature range and showed an emission at 1.55 µm wavelength at room temperature. These results confirm a great promise for InAs-InP QR-NWs for telecom-band lasers monolithically integrated on silicon substrates for photonic chips.

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Abstract ID: 174

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Industrial applications of composite materials

Keywords: Fly and bottom ashes, Power plant, Calcium carbonate, CO2, X-ray diffraction, X-ray photoelectron spectroscopy, and principal component analysis

Ashes characterization to reduce CO2 emissions

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The operation of thermal power plants for electric energy production implies the generation of heat from coal, oil or other fuels to produce water vapor. The use of fuels produces ashes. Dry and wet fly ash (CSV and CHV) and dry bottom ash (CSF) are by-products of coal power plants and resulting from the combustion of pulverized coal used as fuel. This residue is constituted by the particles that leave the boiler carried by the burnt gases. Ash accounts for 10% of charcoal burned. The grain size of the ashes ranges from 0.5 to 300 micrometers. To avoid pollution, retention is doing before the gas is released into the atmosphere by electrostatic dust separators, and cause large amounts of ash deposited in the land adjacent to power plants. The quality of the ash depends on the fineness, the chemical composition and the mineralogical composition. Silica-alumina ash is produced from bituminous coal and are important because of its pozzolan properties. Sulfur-calcic ashes are produced from lignite and among other minerals have gypsum and calcareous, giving as residue of combustion, calcium sulfate and calcium oxide free. This study offers a promising ashes to reduce CO2 emissions of greenhouse gases. The results showed that the highest percentage of Ca, O, and C were CSV with respect to CHV, CSF, due higher content of Ca. The analysis by XPS shows possible combinations of Ca2p3 in the presence of the different elements, considering in this case only the C1s, O1s and Si2p, since these resulted bituminous samples as shown in CSF ashes. The CaCO3 compound was presented in the ashes, as do the studies of XRD and EDS, it has the crystalline structure of compound, and XPS checks that the surface is still present.

Key Words: Fly and bottom ashes, Power plant, Calcium carbonate, CO2, X-ray diffraction, X-ray photoelectron spectroscopy, and principal component analysis

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Abstract ID: 175
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Polymeric composites
Keywords: polymer, capacitive sensor, foams

Soft and highly sensitive capacitive pressure sensors array based on a polymeric foam

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Flexible low-pressure sensors have raised a lot of interest in the past ten years for their promising applications in health [1] (such as biomonitoring and electronic skin) but also as tunable electronic devices that could be used both in sport and industry [2]. We present here an unconventional capacitive pressure sensor, based on a polymeric foam filled with conductive carbon black particles. We design a new material by preparing a PDMS porous material of closed porosity by using an emulsion road [3]. The surface of the closed pores is covered by carbon black conductive particles. These materials have very high permittivity

(r=1000 at 10 hz) and display large electrostrictive coefficient. The sensors made by using these materials are low-cost, highly sensitive at low pressures (S = 5 kPa-1 for pressures < 1 kPa) [3] and particularly versatile. We show that they can easily be built in arrays of varying shape and size with a simple adaptation of the bottom electrode, and their sensitivity is tuned by varying the thickness of the polymeric foam and their geometry. In particular, we build a 4x4 cm2 array of 25 sensors, and use it to measure the small (<500 Pa) and localized pressures which develop in the flow of complex fluids. The sensors are placed either on the plate of a classical rheometer, or used to measure the forces arising during the spreading of a liquid on a soft substrate. We demonstrate that pressures as small as 5 Pa can be easily detected, which allows us to build a 2D mapping of the local pressure. Beyond obvious applications in industry, the versatility of our devices make them particularly promising in sports, for example for smart shoe insoles.

Key Words: Low-pressure sensor, flexible electronics

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Abstract ID: 176

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Nanogenerators and self-powered nanosystems

Keywords: Energy harvesting, electrostriction, dielectric composites, carbon, cantilever.

Integration of electrostrictive bilayer composites into cantilever systems for mechanical energy harvesting

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Different transducers (electromagnetic, piezoelectric or electrostatic systems) are studied for decades to convert vibrational energy into electricity. But they suffer from several limitations, including difficult integration, brittleness, low efficiency or large electric losses. New energy harvesters are emerging, exploiting triboelectricity [1] or electrostriction [2]. As triboelectric systems are very sensitive to humidity [3] and present large impedances [4], studying other transducers as electrostrictive systems makes sense. Indeed, the flexible and stretchable nature of electrostrictive polymers makes them good candidates for developing highly sensitive generators, with greater integration ease. We design a new material by preparing a PDMS porous material of closed porosity by using an emulsion road [5,6]. The surface of the closed pores is covered by carbon black conductive particles. We use the material as a dielectric layer in a capacitance whose value varies due to the vibration of a cantilever. This induces back and forth displacement of electrons and thus production of energy along a cycle. We are demonstrating that this structure provides a positive energy balance thanks to a non-conventional bilayer structuration of the active material. We measured a net power of 2.8 for an acceleration of 3 g and a frequency of 25 Hz under a low bias voltage of 64 mV/. The low resonant frequency of the triangular cantilever, makes the device promising for ambient energy harvesting. In addition, the low-cost process and low toxicity are criteria encouraging their future development.

Abstract ID: 177

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Nanostructured materials for advanced batteries

Keywords: Hetero-nano-structure, Nano, Energy harvesting, Meta-material, Nuclear battery

Meta-material made super-capacitor that harvests nuclear particles kinetic energy and delivers it as electricity

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Energy released in nuclear reactions is by one million times larger than that delivered in chemical processes, and using engineered nano-hetero structures it become possible to produce battery like systems. There are three types of batteries that can be produced, generically called:

- isotopic batteries, known for using nuclear transmutation reactions that release alpha or beta radiation, that is harvested and converted into electricity, previously known as alpha or beta voltaic, one such battery delivering the energy of more than 100,000 same power chemical batteries.

- fission batteries, delivering energy at demand, being in fact a solid-state compact nuclear reactor, where the meta-material inside is harvesting the energy of the fission products , which are over 200 times more energetic than decay reactions, and

- fusion batteries, where the meta-material is harvesting the energy of the fusion reactors, where fusion is up to three times more energetic than fission.

Complementary these meta-materials may be morphed on surfaces, able to convert particle beam energy, useful in space beamed power applications, and being hyperbolic meta-structures for some combinations they exhibit intense EM properties, being possible of emitting THz up to optical radiation.

There are many functional configurations of meta-materials that may be used, to convert moving particle energy into electricity as:

- planar structures, made of parallel nano-layers of materials , where for harvesting the energy of a 3 micron thick alpha emitter, as 210Po, 239Pu, 241Am, it takes a harvesting double foil of about 50 mm thick, useful for self-powered electronic modules, or long term batteries. For example using 40 g of pore 238Pu, it may produce a 200 g, 40cc, 15 W battery, able to power an artificial hart for more than 40 y, or 400 y lifetime batteries for space applications by using 241Am. In a modified configuration, the meta-material may work similar to a laser emitting THz or visible radiation for the same lifetime for data communication purposes.

- nano-beaded structures, made of a distribution of nano-beads embedded into an amorphous dielectric structure, that have higher operating temperatures and efficiencies than planar structures, and

- heterogeneous nano-tube structures, believed to exhibit higher conversion efficiencies, over 90%, for isotropic radiation, but exhibiting real constructive difficulties, being now only a theoretical endeavor.

The project is in TRL=3 stage, having some simulations and ion beam tests accomplished, and more work is needed to develop the highly functional and reliable power sources.

Abstract ID: 178

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Quantum dots, strain reducing layer, ITU band, optical properties

Structural and optical properties of wavelength tunable InAs/GaAs QDs optically active at O-band telecommunication window

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The III-V semiconductor quantum dots (QDs) are attractive physical subjects demonstrating unique physical properties and their potential for applications in micro- and optoelectronic devices. These nanostructures are fabricated by means of the Stranski-Krastanov (SK) growth mode, which is driven by a lattice mismatch between the dot material and the capping material. There are some significant drawbacks to the standard SK growth mode which have motivated research into alternative approaches for QD formation. Two such challenges involve the random location and size dispersion of the QDs grown by this technique. The main objectives of this work is reach better homogenization of the QDs nanostructures grown by solid source molecular beam epitaxy (SS-MBE) for increasing their emission wavelength by varying the strain around QDs using InGaAs strain reducing layer (SRL). By combining the structural and optical studies such as, PL, EPL, TRPL, and Raman spectroscopy, a different approach of (In)GaAs strain reducing layer combined with InAs QD have been investigated. In particular, the international telecommunication union (ITU) band can be reached by varying the (In)GaAs surrounding material, which is particularly interesting for the fabrication of emitters in the telecommunication band and should be useful for the industrial development of today's nanotechnology.

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Abstract ID: 179

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: Surface Acoustic Waves, Exfoliation

Ultrafast Acoustofluidic Exfoliation and Manipulation of Transition Metal Dichalcogenide Crystals

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2D crystalline materials possess outstanding performance for application in electronics, energy and catalysis, however, their realization pivots on the ability to exfoliate them from a 3D bulk down to monolayers. However, this goal remains elusive particularly in terms of a rapid processing method that facilitates high yield and control over the material dimensions, while preserving high crystal quality. In this talk, we uncover an ultrafast exfoliation mechanism that exploits the piezoelectric nature of a number of these materials and that involves triggering electrically induced mechanical failure across the weak domains of the material. In particular, we demonstrate that microfluidic nebulisation using high frequency acoustic waves exposes a bulk 3D crystalline piezoelectric material such as molybdenum disulphide (MoS2) and tungsten disulphide (WS2) to a combination of a large mechanical and electrical fields. These large mechanical accelerations exceeding 108 m/s2 and applied electric fields surpassing 108 V/m rapidly cleave the materials into nanosheets comprising mainly single layers, thus constituting a continuous method, with high-throughput yet on a miniaturised chip-scale that opens new possibilities for scalable production and spray coating. In addition, these acoustic waves are shown to modify the Photoluminescence and bandgap properties of single as well as odd layered MoS2.

Abstract ID: 180
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Smart Composites
Keywords: Nano, Dynamic Composite, Auxetic, Structural Hierarchy

Polymer nano-composites as functional building blocks for dynamic composites

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Despite over 30 years of extensive research exploring the wealth of nano-composite formulations, the understanding of how the nano-scale originated properties can effectively be transferred to the large-scale behavior of hierarchically architected composite structures remains in its infancy. The understanding of fundamental principles of structural composites along with geometrical build up patterns of mechanically robust biocomposites and structural architecture of auxetic metamaterials is the foundation of a novel dynamic composite design paradigm. Fabrication of dynamic composites, exploiting these fundamanetal principles, requires mechanically robust, assembly information rich building blocks and function specific hierarchical build up principles all synthetically programable on the building blocks level. The foundational challenge is a facile preparation of structurally and functionally coded building blocks architected at different length scales and possessing prescribed cross-scale connectivity. Polymer nano-composites with controlled spatial organization of nanoparticles represent technologically viable candidates enabling facile fabrication of the desired building blocks with dimensions and structures architected at multiple length scales. However, the large span in length scales and the overall complexity of dynamic composites impose a combination of requirements, which are well beyond the reach of the existing technologies.

Recent experimental results and computer simulations will be presented on dynamic composites with gradient of auxetic behavior based on nano-scale building blocks assembled into dynamic composite structure employing a cascade of equilibrium and non-equilibrium fabrication processes. Preliminary results suggest, that nano-scale building blocks can synthetically be programmed to rapidly form desired assemblies in a monomer using external stimuli. Combining this local nano-structure control with robust frontal polymerization in a simple 3D printing technology enables the merger of the function-specific nanostructured detail with facile high volume manufacturing. Our results provide some leads for the development of novel dynamic composites combining engineering properties with adaptability. These dynamic composites will instigate a paradigm shift in the design and fabrication of shock resistant aerospace objects, lightweight armor and blast protection structures, protective sport gear as well as mitigate seismic hazards and vibrations of large machinery.

Key Words: Nano, Dynamic Composite, Auxetic, Structural Hierarchy

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Abstract ID: 181

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Anodes and cathodes Materials

Keywords: HER, TMDCs, EC-STM

Exploring the Flatland of 2D materials by Electrochemical STM: visualization of active sites in operando conditions

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2D materials such as chemically modified graphenes, transition metal dichalcogenides, layered double hydroxide to name only a few, are having a huge impact on electrocatalysis providing materials with outstanding activity for a variety of reactions.[1]

However, despite the intense research efforts in this field, a clear identification of the real active sites in many reactions remains a great challenge, given the necessity to employ spatially and structurally sensitive techniques in operando conditions (i.e. during the application of an electrochemical potential in the presence of an electrolyte).

Here we present an innovative approach to the study of 2D materials by using electrochemical Scanning tunneling microscopy. As demonstrated by a seminal paper,[2] this technique allows identifying the presence of catalytic processes at the nanoscale by observing a typical noise in the tunneling current, which is due to instantaneous variations of the tunneling junction.

By using special model systems consisting of CVD grown transition metal dichalcogenides thin films (MoSe2 and WSe2), we achieved even atomic resolution during the hydrogen evolution reactions. This allowed us to distinguish the chemical activity of several chemical and morphological features such as single atom vacancies, step edges, and even exotic line defects such as metallic twin boundaries.[3]

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Abstract ID: 182

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Design and application of composite structures

Keywords: silver lignin nanoparticles, antibiofilm enzymes, self-defensive layer-by-layer coatings, antibacterial activity

Nano-enabled multilayer coatings with switchable bacteria-killing activities for prevention of catheter-related infections

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Medical device-associated urinary infections are the most common healthcare related infections accounting for increased morbidity and mortality, prolonged time of hospitalization and huge financial burden on healthcare services. More than 80% of such infections are due to antibiotic resistant biofilm formation, whereas approximately 40% of all hospital acquired infections are catheter-associated urinary tract infections (CAUTIs). Current strategies to reduce CAUTIs include often replacement of the device, which causes considerable discomfort to the patients and increases the treatment costs, or aggressive antibiotic therapies with associated side effects such as hypersensitivity, inflammatory responses and development of drug resistant bacteria. Alternative solutions for effective inhibition of bacterial growth and biofilm establishment on catheters are urgently needed to improve the patient quality of life, safety, and catheters´ life-span. In this study, we engineered self-defensive nano-enabled coatings with bacteria-triggered antibacterial activity using layer-by-layer self-assembling approach. Hybrid lignin capped silver nanoparticles (AgLNPs) with high antibacterial activity against a panel of medically relevant Gram-positive and Gram-negative bacterial pathogens were synthesized and used as both functional and structural element in the assembly of the multilayer coatings containing bacteria-degradable elastin and anti-infective/antibiofilm enzyme acylase. The enzyme in the uppermost layer attenuated the virulence of the Gram-negative Pseudomonas aeruginosa and inhibited its ability to form resistant biofilms by 90 %, while the triggered release of AgLNPs resulted in total bacteria elimination at lower bactericidal concentrations. These multilayered coatings were biocompatible to human cells and therefore offer potential for addressing catheter related bacterial infections with minimized side-effects.

Abstract ID: 183

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: Smart mesoporous silica nanoparticles, biofilm-degrading enzyme, stimuli-responsive nanosystem, drug delivery, biofilm eradication

Enzyme-decorated mesoporous silica nanoparticles for elimination of antibiotic resistant Pseudomonas aeruginosa biofilms

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Bacterial antibiotic resistance is frequently associated with their ability to form biofilms, acting as a physical barrier that limit the antibiotics penetration and bacterial eradication. Most of the existing strategies aim to inhibit bacterial growth and prevent the biofilm formation, but they become ineffective once the biofilm is well-established. Herein, stimuli-responsive mesoporous silica nanoparticles (MSNPs) were developed for treatment of antibiotic resistant Pseudomonas aeruginosa (P. aeruginosa) biofilms. In this smart delivery nanosystem, imipenem was loaded inside the pores of MSNPs using high intensity ultrasound and then coated with elastin, which was used as stimuli-responsive gatekeeper degraded by P. aeruginosa elastase in biofilms. Subsequently, poly(ethylenimine) and biofilm matrix-degrading enzyme alginate lyase were deposited onto the MSNPs using Layer-by-Layer strategy. At the site of biofilm infection, the enzyme broke down the biofilm matrix and allowed the penetration of the antibiotic loaded MSNPs into the biofilm structure. Then, the P. aeruginosa triggered the controlled release of the antibiotic resulting in bacterial elimination and prevention the formation of new biofilm. The developed stimuli-responsive MSNPs exhibited up to 80 % eradication of total biomass and 4 logs bacterial cells viability reduction in already established antibiotic resistant biofilm. These smart MSNPs possess 100% biocompatibility and provide an efficient platform for prevention and treatment of P. aeruginosa biofilms.

Abstract ID: 184

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Magnetic Polymer

Keywords: ladder polymer, pi-conjugation, thermoresponsive materials, Pauli paramagnetism

Organic Functional Materials Derived from Rigid Ladder-Type Molecules and Macromolecules

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Conjugated ladder-type molecules and macromolecules represent an intriguing class of organic compounds featuring rigid pi-backbone and promising potential applications as functional materials. In such a structure, the coplanar molecular conformation facilitates the delocalization of not only molecular orbitals, but also possible charges, excitons, and spins, leading to synergistically ensembled properties of the entire conjugated system. A rigid backbone, meanwhile, imposes a low entropy of the system and a high energy cost to disrupt such a favorable conformation, ensuring the robustness and persistence of coplanarity. From a supramolecular and material point of view, coplanarity and rigidity often promote strong intermolecular electronic coupling and reduce the energy barrier for the transport of charges, excitons, and phonons, affording advanced material properties in bulk. This talk describes our effort in the design, synthesis and processing of novel conjugated ladder-type organic materials. By taking advantage of their unique constitutional and conformational structures, we demonstrate the promising applications of this class of materials in terms of thermoresponse, electronics, Pauli paramagnetism, gas adsorption thermodynamics, etc.

Key Words: ladder polymer, pi-conjugation, organic electronics, gas adsorption, thermoresponsive materials, Pauli paramagnetism

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Abstract ID: 185

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Gas Sensor, Ozone, Nitrogen Dioxide, Nano, Palladium (II) Oxide

Homogeneity Region of Palladium (II) Oxide Nanocrystalline Films for Gas Sensors

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Low level ozone which is a product of industrial activity, transportation, etc., has been accumulating at the surface of the Earth during the last twenty five years. WHO and US EPA declared that ozone O3 and nitrogen dioxide NO2 could be very dangerous for human health especially for children, the elderly, and patients with lung diseases [1]. Pollution of ambient air with low level O3 and NO2 is a serious problem owing to cyclic processes of these gases via mutual transformation under sunlight [2]. Interaction of O3 and NO2 with volatile hydrocarbons produces many toxic organic substances as a result of oxidation reactions. Palladium (II) oxide nanostructures were employed for O3 and NO2 detection. Homogeneous nanocrystalline PdO films (with thicknesses ranging around 10, 35, and 100 nm) with p-type conductivity and energy band gap Eg ~ 2.3 eV were prepared on polished poly-Al2O3, SiO2/Si (100), optical quality quartz, and amorphous carbon/KCl substrates by deposition of pure Pd metal layer and subsequent thermal oxidation in oxygen atmosphere at temperatures T = 620 - 1070 K. It was established that nanocrystalline PdO films have the high sensitivity, operation speed, stability, short recovery time, and good reproducibility of sensor response [3, 4]. In this work by XPS measurements it has been found that PdO nanocrystalline films contain a small concentration of palladium atoms in oxidation state (+4). The composition of PdO films within the homogeneity region is one of key parameters which determine the sensitivity toward the toxic gases with the oxidative and reductive properties [2]. The precise XRD experiments have shown that the lattice constants of the tetragonal crystal structure of homogeneous nanocrystalline PdO films increase with the rise of oxidation temperature up to T = 1020 K. On the basis of the unit cell volume values of PdO films prepared at temperatures between T = 620 - 1070 K and well known values of Pd (2+), Pd (4+), and O (2+) ionic radii the width of homogeneity region has been calculated. It has been found that nanocrystalline PdO films have excess of oxygen atoms from the stoichiometric ratio.

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Abstract ID: 186

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Theory of graphene, Mxenes and other two-dimensional materials

Keywords: transition-metal dichalcogenide monolayers; density functional theory; band structures, spin-orbit coupling; nonequilibrium Green's function

Designing Electronic Devices at Nanoscale by tuning the Optoelectronic Properties of Monolayer transition metal Dichalcogenide and alloying

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From the time of graphene discovery by Geim et al. in 2004 [1], research on atomically thin two-dimensional (2D) materials have acquired increasing interests in wide fields of frontier science because of their widespread potential applications in optoelectronic and electronic devices. Alternately, single layered transition-metal dichalcogenides (TMDCs) [2] have generated great interest owing to their promising physical functionalities and for applications varying from nanoelectronics and nanophotonics to sensing and actuation at the nanoscale [3]. TMDCs, with a general structural formula named MX2, where M symbolizes for a transition metal (e.g., Mo. W) and X for chalcogen atoms, have a typical three atomic layer structures and direct band gap semiconductors (with an optical band gap of 1-2 eV), which can be either exfoliated or grown with chemically stable surfaces. We performed different computational investigations of electronic, optical, properties of monolayer transition metal dichalcogenides by employing first principle calculations. We reported lattice constants, bond lengths for MoSe2 and MoTe2 and their alloy Mo(Se0.5Te0.5)2. From the band structures analysis of the monolayer alloy, we have gained useful information about the more dispersive nature of their conduction bands with respect to their valence bands, causing the band gaps to lower and increase in electron effective masses. Optical properties acting as imaginary and real parts of dielectric function, have been discussed in consideration of change of concentration. Furthermore, the transport properties of Mo(Se0.5Te0.5)2 alloy monolayer were calculated by density functional theory schema mingled to non-equilibrium Green's function approach. We reported the transmission for zero bias and discussed its features in light of the projected local densities of states. The device I-V curves were also reported by discussing the effect of the voltage applied across the metal dichalcogenides electrical device and the current flowing through it. The present theoretical study open routes for exploring nano-devices for optoelectronic and photovoltaic application by tailoring their band gaps and constructing different architecture at nanoscale level.

Key Words: transition-metal dichalcogenide monolayers; density functional theory; band structures, spin-orbit coupling; nonequilibrium Green's function

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Abstract ID: 187

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Multifunctional composites

Keywords: CMET, Bio-active monomer, adhesive monomer, Odontoblast-differentiation

CMET, a bio-active adhesive monomer, induces odontoblast-differentiation in vitro

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In current adhesive dentistry, the development of multifunctional materials possessing not only high adhesion performance and mechanical property but also remineralization activity, antibacterial action and so on. It is an important issue for improvement of the durability of dentin-bond interface. We previously reported that CMET1,2), calcium salt of 4-MET, induces dentin remineralization in vitro, and it significantly promotes shear bond strength to dentin, bending strength and compressive strength of resin-based coating material. It is necessary for increasing added value of CMET in adhesive materials to search for its further functions. The purpose of this study was to evaluate the effect of CMET on odontoblast differentiation in vitro.

MDPC-23 cells were used in cell culture. CMET was first dissolved in dH2O with the concentration of 10 mg/mL, then the different concentration of CMET was added into experiment group. dH2O was served as blank control, 4-MET was used as a negative control, Ca(OH)2 and MTA were employed as positive control. Cell proliferation was assessed using CCK-8 assay. ALPase activity and qPCR was carried out on day seven of culture. Finally, the mineralization inducing capacity was evaluated using alizarin red staining on day eight. Statistical analysis was conducted using One-way ANOVA with post-hoc Tukey HSD Test.

The addition of CMET promoted the proliferation of MDPC-23 cells, high concentration of CMET did not cause apoptosis compared to Ca(OH)2 and MTA. The mRNA expression of rCOL1A1, rOCN was up-regulated in CMET treated group. Moreover, the gene expression of rDMP-1, rDSPP, and rOPN was strongly enhanced by CMET. Finally, the mineralization of MDPC-23 cells was significantly strengthened by the addition of CMET, the promoting effect was in a dose-dependent manner and comparable to Ca(OH)2 and MTA.

The findings indicate that CMET promoted proliferation, odontogenic differentiation and mineralization of MDPC-23 cells in vitro, though its detailed mechanism needs further study.

Abstract ID: 188
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Porous and cellular materials
Keywords: IGCC Slag, Si Sludge, Porous Geopolymer, Microstrucrure

Mixing Effect of Slurry of Porous Geopolymer with IGCC Slag and Si Sludge

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Integrated gasification combined cycle (IGCC) slag from power plant and Si sludge from Si wafer processing company were used as raw material and bloating material for lightweight porous geopolymer which is considered as one of prospective building materials for replacing traditional cement. A rapid and furious exothermic bloating reaction by adding small Si sludge addition occurred during the mixing process of slurry of IGCC slag, Si sludge and alkaline activators. This bloating reaction brought a drastic volume expansion by forming pores inside of the slurry so that the microstructure and property of geopolymer could not be controlled in the manufacturing process. An extra-mixing in the middle of bloating reaction during molding was introduced to control the microstructure and to enhance the property of porous geopolymer. The optimum extra-mixing time was different according to the water/solid (W/S) ratio of slurry and it is difficult to determine because there is no such an engineering criterion for proper extra-mixing time during the bloating reaction of geopolymer; however, specimens processed after 10-20 minute extra-mixing showed a more homogeneous pore size and distribution compared to those without an extra-mixing process. When the W/S ratio was 0.22 with 2.0 wt.% Si sludge addition, the specimen with 20 minute extra-mixing time during molding showed the best pore distribution with 1-3 mm pores which is much smaller than those (1-20 mm) without extra-mixing process. The density of the specimen increased from 0.4 to 1.2 and the compressive strength increased from 1 MPa to 10 MPa. It is believed that the increase in both density and compressive strength was resulted from the change of microstructure of gepolymer by introducing an extra-mixing process. An engineering criterion for extra-mixing process must be secured in the nearest future for applying this process to manufacturing process in practice and the limit of Si sludge addition will be also determined in the future research.

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Abstract ID: 189

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Keywords: CdSe Quantum dots; chemical bath deposition; X-ray diffraction; Optical properties

Influence of deposition time on Structure, optical and electrical properties of nanocrystalline cadmium Selenide thin films prepared by chemical bath deposition method

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Influence of deposition time on Structure, optical and electrical properties of nanocrystalline cadmium Selenide thin films prepared by chemical bath deposition method

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Abstract:

CdSe Semiconducting thin films with a mean diameter of 20 nm are synthesized using a simple chemical bath deposition (CBD) method on glass substrate at temperature 70°C . Chemicals used for the deposition of CdSe thin films were cadmium chloride salt CdCl2, sodium sulphate (Na2SO3), selenium metal powder (Se), ammonia solution (NH4OH) (25%), and hydrazine hydrate (N2H2, 2H2O). The influences of deposition time are investigated (60, 80, 100, 120 minutes) . The structural and optical properties of CdSe thin films are studied using X-ray diffraction and UV-visible absorption spectroscopy. The X-ray diffractions study showed that all the films were polycrystalline in nature having a cubic phase with zinc blende structure with prefer orientation along (002) plan. Optical properties are studied shows blue shift in peak position were observed for films deposited at different deposition time. The optical studies reveal that these thin films have direct allowed band gap energy ranging from 2 eV to 2.9 eV. The band gap energy increases with increases the deposition time. The electrical analysis shows that the electrical resistivity is observed to be decreased with thickness. because of well-crystallized, high transmittance in visible region (> 80%) and wide band gap values the deposited CdSe thin films were suitable for many optical devices, such as solar cells

Keywords: CdSe Quantum dots; chemical bath deposition; X-ray diffraction; Optical properties

Abstract ID: 190
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Multifunctional composites
Keywords: Nano, Nuclear-Energy, micro-hetero structure, nano-clustered-hetero structure

Composite micro-nano-hetro-structures for nuclear power applications

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Nuclear power as we know today has embedded difficulties that finally translated in many accidents and an increase in cost of the energy delivered this way. Main problem is the accelerated degradation of nuclear fuel under the action of fission products, transmutation products and radiation inside the active zone, corroborated with improper temperature distribution and mechanical stress induced during operation.

The searches to solve these problems conducted to development of micro-nano-hetero structures able to use nuclear reaction kinematics to self separate the fission products from the nuclear fuel in microstructures, generically called “Cer-Liq-Mesh”, made of nuclear fuel (UO2, PuO2, UN, PuN, PuC, etc) micro-beads, with dimensions inside fission products range, chemically stabilized by a thin coating, soaked in liquid metal fluid. In order to assure mechanical stability the micro-beads are suspended on a wire mesh, or felt that is also elastic. As further analyzed, fission products share about 170 MeV in kinetic energy, and in interaction with the matter surrounding the fission origin they behave like charged particles depositing energy as ionization and nuclear recoil towards the end of the stopping range. In solid matter the nuclear recoil zone, also known as Bragg peak is characterized by having many remnant defects as dislocations. The new solid-liquid composite material, places Bragg peak in liquid, that has exhibits no remnant structural damage.

Transmutation products have shorter stopping range in nuclear fuel in nm range, and in order to extract them, a nano-clustered porous hetero-structure have been developed, where the pores are open and flooded with an extraction fluid, acting as a drain liquid. Nano-cluster exhibit special properties [1] for impurities, different from bulk material, that makes a transmutation product created inside a nano-cluster to be expelled on the boundary from where the extraction liquid washes it out. In an ideal case, the micro-bead may be made of a nano-clustered structure contained inside the coating layer together with the extraction liquid.

This type of nuclear fuel material that contains a porous nano-clustered structure embedded or forming a micro-hetero structure allows the separate extraction of the fission products from the micro-fluid and transmutation products from the nano-fluid may be packed together inside a cladding creating fuel pellet, that may be fully compatible and replace the actual nuclear fuel. The advantage is that after a reasonable burnout, the fission or fission and transmutation products may be extracted on spot and the fuel may be reprocessed pellet by pellet, transferred in a new cladding and used in a breed and burn scheme, reducing the need for enrichment, and by this improving the nuclear fuel cycle and nonproliferation resistance.

Abstract ID: 191

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices
Keywords: Carbon materials, geometric and electronic effects, OPNS, new catalyst.

Theoretical strategies and Methodologies for Investigating Electrocatalytic Reaction (HER/OER/ORR/IRR) on Carbon-based Nanostructures

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Carbon materials doped with heteroatoms have demonstrated significant interest as electrocatalyst because of their tunable surface chemistry and fast electron-transfer capacity but remains challenging to suggest theoretical insights for high-performance. Through the recent developments of various carbon-based 2D materials (P, S doped C3N4[1], S doped C2N[2] and Mn, Fe doped MOF[3]), we have suggested and emphasized the synergistic effect between geometric and electronic effect of that catalysts, which result in the improved catalytic activities. Generally, the large heteroatom leads to structural deformation by inducing sp3 hybridization to active sites in the deformed region. These sp3-C sites compared to sp2-C sites can efficiently promote chemical bonding with intermediates of various catalytic reactions. Based on its structural factor, we have remarkably activated abundant carbon sites of existing inert catalysts, and suggested that forming proper concave and convex region via doping plays an important role in improving the catalytic activities. Moreover, such doping approach can improve the conductivity as a consequence of modification in electronic structure. The p- and n-type doping effects are expected from electron deficient and rich elements, and this plays a crucial role in converting semiconducting into metallic material with increased conductivity. Consequently, these two effects can provide suggestive insights for enhancing the catalytic activities of carbon materials. In addition to, we proposed a new methodology called “one probe and non-equilibrium surface Green’s function (OPNS)” to shed light on the longstanding controversial issue of the catalytic reaction mechanisms.[4] With aid of OPNS overcoming the limitations of free energy diagram using theoretical slab model, we clearly elucidated that the catalytic reaction mechanisms are significantly dependent on the external electric field, not the adsorption strength of intermediates that has been theoretically asserted thus far. This study can be a good tool for uncovering reaction mechanisms of various conventional catalysts, and can motivate the study for designing a new catalyst with high catalytic performance.

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Abstract ID: 192

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster/Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Flexible organic crystals, organogels, luminescence, optical waveguide

Modulation of Mechanical and Luminescence Properties of BORANILs through Sidechain Engineering

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Macromolecule-based organic materials have found wide-spread application in optoelectronics because of their flexibility and tuneable properties. However, small organic molecules lack the mechanical properties needed for device fabrication and require a supporting matrix. Generally, single crystals are brittle and inelastic thereby limiting their use in flexible optical and electronic devices. Flexible organic crystals are emerging as new materials in this direction. Initial advances in this field suggests that a packing pattern consisting of interlocked molecules through weak and dispersive interactions would result in elastically bendable crystals whereas structural anisotropy arising from slip planes leads to plastically bendable crystals.[1] However, it is too early to generalize the design principles because examples of organic crystals that do not follow the above design rules have also been reported. We have synthesized a series of BORANIL molecules by the complexation of Schiff bases with boron (III). Our results indicate that mechanical properties of the molecules can be varied from rigid, brittle crystals to flexible crystals and to organogels through subtle variations in the sidechains. Moreover, the BORANILs exhibited excellent luminescence properties including optical wave-guiding which could further be modulated through supramolecular interactions with entrapped dye molecules.

Abstract ID: 193

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Metamaterials and Materials for THz, Plasmonics and Polaritons

Keywords: THz, detection, imaging, Micro, Nano, EM resonances, eigen-modes

Molecular band THz detection and imaging structures

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Chemical compositions have molecular vibration eigen-modes in THz region and are emitting and absorbing EM waves in this region with wavelengths between 1 mm and 1 mm overlapping in part the thermal emission. The present technology to emit and receive THz waves is bulky and requires complex devices. Integrating conductive microstructures embedded in metal oxides and conducting micro-spheres that creates a voltage parametric amplifier of resonant bands with a FET transistor structure makes possible to create a THz line detector having the size by one order of magnitude bigger than the detected wavelength.

In order to positively identify a molecular species, a plurality of such detectors have to be used together, in order to cover all spectral bands that molecule may emit or not. Supporting the metal structures on piezo-electric materials is possible to tune the resonant frequency of the detector in a larger band and associating several detectors together to be able to scan all THz spectrum producing a direct molecular identification. Further we may tune on a selected substance and using a scanner or a plurality of detection sets to produce a 3D image of the selected substance on a specific timeline, being able to record “chemistry in action”.

Because the actual electronics operating frequencies are in GHz domain, at best, and the energy of a THz photon is in meV, it can not be directly detected by photonic devices, we use the perturbation its associated EM wave is inflicting over a differential nonlinear set of FET running a reference signal in GHz or MHz domain, connected to a differential amplifier and a fast, ADC converter connected to a fast direct memory access architecture, shared with a processing computing structure. There are various technological limitations that accounts for various constructive solutions, and the optimization process depends on the application.

Most of the current applications as medicine, chemistry, environment does not require ultra fast imaging and the effort is moved towards the complexity of substances simultaneously present in the area of interest. It has to be noted that THz frequencies have considerably large skin depths in most of materials, except the absorption bands, and in-depth imaging of various bodies may be produced. There is a large palette of applications from security systems to medical, engineering and research systems.

Abstract ID: 194

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Manufacturing and formation techniques

Keywords: Tubes, Welding, Testing

Dissimilar tube transition joint fabrication by layer by layer metal deposition by using an external tool

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At present small diameter tubing, defined as round tubing, is used in a variety of industrial applications. Tubes are extensively used in almost all engineering industries, and the demand for joining of tubes of dissimilar metals is more in industries including aerospace, nuclear, chemical, petroleum, automobile, and power.

The joining of tubes of dissimilar metals is essential to achieve either improved performance or to reduce the material cost or both. For joining of small diameter tubing, orbital welding has become the preferred joining method. Orbital tube welding is generally a fusion process in which the edges of the joint are melted and fused without the addition of filler material. However, this method is generally not suitable for dissimilar metals due to the formation of brittle intermetallic compounds at the joint interface.

Dissimilar tube transition joint fabrication by layer by layer metal deposition by using an external tool is invented by the present author and an Indian patent has been filed (Application No. 201741041008 dated 16-11-2017) [1]. This process is capable of fabricating dissimilar metals transition joints, and the process is more economical compared to other processes.

In the present research, transition tube joints between AA1050 and AA 6061 are fabricated by layer by layer metal deposition by using an external tool method, and mechanical and metallurgical properties are studied. The results show that the dissimilar tube transition joint fabrication by layer by layer metal deposition by using an external tool is a versatile technique having high potential industrial applications.

Abstract ID: 195

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Nanogenerators and self-powered nanosystems

Keywords: Triboelectricity, Particulate matter, Dielectric material, Adhesion, Hydrophobicity

Influence of electrostatic film structure on particulate matter adhesion

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As air pollution problems such as particulate matter (PM), exhaust gas, and yellow dust become more serious around the world. And various environmental regulations such as EURO-6 and SULEV (Super Ultra Low Emission Vehicle) are gradually being tightened. Among them, PM, designated by the World Health Organization (WHO) as a first-class carcinogen, has a particle size of 1/10 to 1/25 of the hair. It is known to have a very harmful effect on our health. In addition, it is regarded as one of the serious environmental problems related to air quality, visibility and climate change, and the social cost to remove a PM is increasing every year. Therefore, there is a need for a method that can efficiently remove PM for living environment and public health. Generally, PM removal is achieved by mechanical dust collection through direct interception, inertial impaction, and Brownian diffusion, using filters consisting mainly of micro- and nano-sized fibers. The PM removal efficiency can be enhanced with using higher surface area of the filter with lower porosity. However, it brings out the pressure loss with energy consumption of the air circulation pump. That is, in the case of PM removal using a mechanical dust collection method, there is a trade-off relationship between the PM collection efficiency and the pressure drop. Therefore, it is necessary to improve the filter technology to remove the PM with low energy consumption. In order to solve these shortcomings, this study introduces a method of capturing PM using static electricity that can be experienced around. A conceptual study was carried out to collect PM without loss of pressure by making it a hydrophobic polymer film with porous structure. In this regard, the electrostatic film has great potential for washable filtration system, and PM removal system.

Abstract ID: 196

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Magnetism and Magnetic Materials

Keywords: Perovskites, Magnetocaloric effect, Universal master curve.

Magnetocaloric effect of La0.9Ca0.1MnO3 perovskite

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Perovskites have generated much interest in the last decades due to their complex and unusual physical properties. In this work, we report our investigation on the magnetocaloric effect (MCE) for La0.9Ca0.1MnO3(LCMO) perovskite, with different methods, hoping to extend our knowledge on the characteristics for refrigeration applications of those systems. The sample has been prepared by solid-state reaction and sintered in the air at 1200 C for 24 hours. The X-ray diffraction pattern confirms of a single phase. Magnetic entropy change (ΔSm) was measured based on the temperature (T) and magnetic field (H) dependences of the magnetization, M(H, T) with T = 50 - 200 K and H = 0 - 50 kOe, determined by the Maxwell's relation. ΔSm reaches the maximum around the ferromagnetic-paramagnetic phase transition temperature with dependence on H, found to be 2.70 J/Kg-1K-1at □H= 50 kOe. Besides, we have applied the Landau's theory, Yamada and Goto have recently developed a method to calculate entropy change. Finally, we have also described the universal master curve for ΔSm, a function of |□Sm|/|□SmP| versus rescaled temperature θ = (T - TC)/ (Tr - TC), where Tr is the reference temperature.

Abstract ID: 197

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Optical properties of metals and non-metals

Keywords: Push-pull chromophores, photonic, charge-transfer, white-light emission

Access to Fluorescent Organic Push-Pull Chromophores with White Light Emitting Property Using Urea as the Electron Donor

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Molecular electronics is being actively pursued in order to miniaturize the electronic world. Organic molecular electronics is promising over inorganic due to unlimited possibility for bandgap tunability, cost effectiveness and easy processability. Conjugated organic push-pull chromophores consisting of Donor and Acceptor functionalities at the terminal positions have been tremendously explored from the past two decades because of their unique features in future generation materials, such as non-linear optical (NLO), Electro-optic piezo chromic materials and solar cells etc.1 Luminescent, in particular white light emitting materials find significant attention owing to their applications in lighting and display.2

Last decade has witnessed a tremendous interest in donor substituted poly-cyano olefins based push-pull chromophores owing to its click type synthesis, high intramolecular charge-transfer (ICT), redox behavior and more importantly with high thermal stability.3 However, due to strong ICT, they generally does not exhibit luminescence. Unlike N,N-dialkylamino group, a bench mark organic donor alkyne,3 Our design strategy offers easy access to further functionalization on these chromophores and exhibits luminescence property apart from the inherent properties like ICT band and redox behavior.4 Herein, we present a new strategy that we adopted to obtain the same. The below figure shows the regardless of weak donor, the push-pull chromophores exhibited white light emission in solution without any complicated composites or conditions, as simple fluorescent organic molecules rarely exhibit such emission.

Abstract ID: 198

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Theoretical and Computational Magnetism

Keywords: Magnetocaloric effect, elastic properties, rare-earth transition metal compounds.

Magnetocaloric Effect, Magnetothermal and Elastic Properties of SmFe3 and ErFe3Compounds

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We report, using the mean field theory, on the magnetothermal properties of the ferromagnetic SmFe3 (Tc ≈ 600 K) and ferrimagnetic ErFe3 (Tc ≈ 600 K, compensation temperature ≈ 230 K) compounds, e.g. the temperature and field dependence of magnetization, magnetic specific heat and magnetic entropy. The Magnetocaloric effect (MCE) i.e. the isothermal change in entropy (ΔSm) and the adiabatic change in temperature (ΔTad) are then calculated using the trapezoidal method and standard relations involving the total specific heat of these systems. The electronic and lattice parts of the total specific heat and total entropy are calculated using the, ab-initio calculated, electronic coefficient of the specific heat γe and the Debye temperature ΘD. The elastic constants, bulk and shear moduli are also ab-initio calculated using the Density Functional Theory, as implemented in the Wien2k code. Both direct and inverse MCE effects are found in the ferrimagnetic ErFe3, while only direct MCE effects are found in SmFe3. Maximum ΔSm, for a 60 kOe field change, is about 1.15 J/mol.K for SmFe3. Maximum direct and inverse |ΔSm| for ErFe3 are around 0.4 J/mol.K for the same field change. The order of the magnetic phase transition in these two system will be discussed in the light of specific features of the thermomagnetic and magnetocaloric properties together with the Arrott plots and universal curves of both systems.

Abstract ID: 199
Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)
Oral Presentation
Topics: Correlated Electrons
Keywords: metallic state, Mott Insulator, cuprates

An emergent metallic state

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Two-dimensional (2D) CuO_2 planes play a key role in high-Tc cuprates. In the present study, ultrathin (1-20 uc) tetragonal SrCuO_2 (SCO) films were successfully layer-by-layer grown on TiO2-terminated SrTiO_3 (STO) substrates using pulsed-laser-deposition technique. The structure of SCO ultrathin films can be controlled. The thickness-dependent structural transformation of the SCO films was studied by polarized x-ray absorption spectroscopy (XAS) at the Cu L-edge, and synchrotron-based x-ray diffraction and Laue diffraction. With the fabrication technology available, we demonstrate a new concept on inducing a 2D metallic phase in the SCO/STO structure via the oxygen sublattice and interface engineering. The electrical transport properties of this new state are studied by the electrical and Hall measurements.

Abstract ID: 200
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Polymeric composites
Keywords: Integrated smart windows, Electrochromism, Energy Storage

Polyaniline-functionalized nickel oxide composite for integrated electrochromic-charge storing smart window application

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Multifunctional smart windows that combine electrochromism with the charge storage ability have recently enticed research.1 Both electrochromism as well as charge storage via pseudocapacitance, work on identical faradic redox reactions, therefore, an integrated device can be deliberately constructed by a wise choice of active smart material fulfilling both the requirements. Such integration opens up new avenues of multifunctional glass windows which can store charge and concurrently adjust the lighting and heating of a building. Inorganic metal oxides like tungsten oxide (WO3), titanium dioxide (TiO2) and Prussian blue, have been studied for this integrated application. However, inorganic materials suffer with drawbacks of low processibility, single coloration and high response time. At the same time, polymeric materials have advantages like higher processibility, ample coloration, fast response, stable memory effect in addition to the flexibility and low cost.2 As far as the charge storing electrochromic devices are concerned, polymeric materials are relatively less explored.

Here in this work a black to transparent efficient electrochromic electrode has been prepared based on functionalized nickel oxide (NiO) and polyaniline (PANI) composite. To ensure strong interaction among NiO and PANI, NiO nanoparticles were first functionalized with (3-Aminopropyl) trimethoxysilane (3-APTS) followed by subsequent attachment to monomer. This linking agent 3-APTS makes a bridge between NiO and PANI. Prepared PANI-fNiO composite exhibits extended contrast throughout the visible spectrum as well as in near-IR and near-UV regions with superior coloration efficiency of 138 cm2C-1 and a very fast response of 1.5s/2s for coloration and bleaching respectively. For smart window applications, such extended contrast throughout the visible spectrum holds an upper hand over contrast at a particular wavelength. The composite PANI-fNiO was found to have improved cyclic stability of 7,000 cycles. Thus with such kind of attachment both components synergistically favor each other's coloration and bleaching, rendering dark (almost) black to transparent electrochromism. Moreover, PANI-fNiO shows pseudocapacitive behavior with a large areal capacitance of 1.1 F cm-2. Both electronic and ionic charge transport mechanisms in such bonded PANI-fNiO composite have been studied using temperature dependent dc conductivity studies, cyclic voltammetery and electrochemical impedance spectroscopy. The observed results present the strong potential of PANI-fNiO composite as an integrated electrochromic electrode with charge storing ability.

Abstract ID: 201

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Dielectric materials

Keywords: Magnetodielectric, Thin Film, Double Perovskites

Magnetodielectric Effect and Interface Couplings in LaMnO3/LaNiO3 Superlattices

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Multifunctional double perovskites, e.g. ferromagnetic insulating La2NiMnO6, have recently gained strong interest because of their rich physics and prospects for technological applications due to the magnetodielectric (MD) effect. To study the origin of MD coupling, epitaxial superlattices of (LaMnO3)n/(LaNiO3)n (LMO/LNO) with n varying from 20 u.c. down to one monolayer (n=1 yields La2NiMnO6) have been grown on electrically conducting Nb-doped SrTiO3(111) at relatively low (Tlow~650°C) and high (Thigh~900°C) temperatures by metalorganic aerosol deposition (MAD) technique, equipped with in situ optical ellipsometry. SLs grown at Tlow show an enhanced exchange bias field, HEB~40Oe, and large coercive fields, Hc~800Oe, as well as a suppressed saturation magnetization (msat,650°C~½ msat,900°C) as compared to those measured for SLs grown at 900°C. This means that the structure of interfaces and interfacial LMO/LNO magnetic coupling may be influenced by growth conditions. Namely, a relatively slow growth kinetics at 650°C seems to suppress the charge transfer between Mn and Ni cations, resulting an enhanced antiferromagnetic coupling between Mn3+ and Ni3+. Taking into account the data of in situ ellipsometry, we further performed measurements of dielectric constant for SLs with n=2, 5 in the temperature range, T=5-400 K, and for frequencies, f=10E-6 - 2*10E6 Hz, to elucidate the role of LMO/LNO interfaces in the MD effect.

Abstract ID: 202

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Ferrites and Garnets

Keywords: ZnFe2O4 adsorbent, Hydrothermal method, As(III) Adsorption isotherms, Treatment of As(III)-polluted water.

Magnetically Soft Nano-sized ZnFe2O4 Ferrite: An Efficient and Non-Toxic Adsorbent for Purifying the As(III)-Polluted Water

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A high concentration of As(III) in contaminated drinking water is continuously posing serious health threats to millions of people worldwide, especially in developing countries. As(III) is abundantly found species in groundwater and is reported to be more soluble, toxic and mobile as compared to As(V). Therefore the affected people especially of rural areas need accessible and simplest technologies for As(III) removal from the drinking water without introducing any toxic/harmful additives in the water body. For this purpose, an attempt has been made to synthesize nanosized magnetic ZnFe2O4 ferrite by hydrothermal method having the advantage of higher saturation magnetization which is beneficial for an easy separation of magnetic adsorbent by applying a moderate external magnetic field. The experimental results showed that adsorption kinetics and adsorption isotherm data were well described by the psudo-second-order and Freundlich models, respectively. The results have also demonstrated that the removal efficiency of the investigated adsorbent remains within the WHO limit even in the presence of most of the competing ions reflecting its good anti-interference capability. In addition, the values of thermodynamic parameters ($\Delta G0$, $\Delta S0$ and $\Delta H0$) at different temperatures suggest that the adsorption of As(III) on the ZnFe2O4 surface is an exothermic, spontaneous and favorable with increasing temperature which might be due to the increased chances of collisions between the reactants (adsorbent and adsorbate). Owing to the appreciable regeneration ability and excellent As(III) adsorption capacity, this adsorbent could be considered as a potential candidate for the treatment of As(III)-polluted water.

Abstract ID: 203

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Optical properties of metals and non-metals

Keywords: Film, Sputtering, Substrate Temperature, Optical Property.

Influence of substrate temperature on the optical properties of hydrophilic SnO–SnO2–Sb2O3 thin films

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A transparent conducting thin film (TCTF) is a vital component of several devices, such as gas sensors, heat mirrors, flat panel displays, photovoltaic solar energy conversion devices, and transparent electrodes. Among various materials for making such thin films, tin dioxide (SnO2) is the most promising because of its good conductivity and transparency in the visible region of the spectrum. Studies of tin monoxide (SnO) are few, due to its metastability with respect to transformation into SnO2 at high oxygen pressure. Increasing the RF power and/or substrate temperature leads to the formation of SnO phase (p-type) and subsequently mixed-phase SnO2 (n-type). The conversion of SnO into SnO2, during the heating process, and the presence of mixed phases (SnO + SnO2) may affect the properties of thin films. Among the physical vapor deposition (PVD) techniques, magnetron sputtering has the advantage of being scalable to large-area on an industrial scale and has been shown to be an efficient way to prepare high-quality films. In this work, SnO–SnO2–Sb2O3 thin films were prepared by simultaneous RF magnetron sputtering of SnO2 and DC magnetron sputtering of Sb. To ensure that the deposited films exhibited nanocrystalline orthorhombic SnO, the RF power density was kept as low as possible. The RF power densities of the deposited films were controlled by modifying an RF power. In addition, the hydrophilic SnO–SnO2–Sb2O3 thin films were obtained in this study. The influence of substrate temperature on the optical properties of SnO–SnO2–Sb2O3 thin films were investigated. Structural changes complicate the characterization of SnO–SnO2–Sb2O3 thin films for optoelectronic applications.

Abstract ID: 204

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Low-dimensional material, 2D Square lattice compound, Oxide materials

S = 5/2 2D square lattice magnet NaMnSbO4

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A new compound, NaMnSbO4, represents a square net of magnetic Mn2+ ions residing in vertex-shared oxygen octahedra. Its static and dynamic magnetic properties were studied using magnetic susceptibility, specific heat, magnetization, electron spin resonance (ESR), nuclear magnetic resonance (NMR) and density functional calculations. When the temperature decreases the magnetic susceptibility demonstrates the behavior typical for low-dimensional magnets with broad correlation maximum at Tmax = 55 K followed by clear anomaly at TN ≈ 44 K, which can be assigned to the long-range magnetic ordering. At the same time unusual character of the TN anomaly and the wasp-waisted hysteresis loop on the magnetization curve indicate that the long-range state is most probably canted antiferromagnetic. ESR spectra of NaMnSbO4 in paramagnetic phase reveal Lorenzian shape signal, which can be attributed to Mn2+ ions and characterized by the temperature independent effective g-factor g = 2.01 ± 0.1. ESR data indicate an extended region of short-range order correlations, typical of low-dimensional or frustrated magnets. An analysis of the ESR line critical broadening performed in the frame of the Kawasaki-Mori-Huber theory confirms low-dimensional character of magnetic exchange interactions in the compound under study. DFT calculations have shown that ground state is stabilized by the five exchange parameters. It was found that all spin exchange are AFM, and that the side exchange J1 on square dominates over all other spin exchanges indicating rather 2D magnetism in new NaMnSbO4 compound. Temperature dependence of the magnetic susceptibility and 23Na nuclear spin lattice relaxation are described reasonably well in the framework of 2D square lattice model with the main exchange parameter J = -5.3 K, which is in good agreement with density functional analysis and ESR data.

Abstract ID: 205

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster/Oral Presentation

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: Graphene, Microbial reduction, microorganism

Microbial Production of Graphene

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Since graphene and graphene-related materials have many uses in every sector from electronics to health, they attract much attention in various fields of science. With the use of these materials and increasing demand from the industry, scientists have begun to look for new, scalable and environmentally friendly techniques to produce graphene. In this study, bacteria called Lactococcus lactis and Lactobacillus plantarum, which can naturally remove oxygen-based molecules from chemicals such as metal oxides, were used for the production of graphene. These bacteria are fed with graphene oxide produced from graphite, which is then converted to graphene by removing oxides. Compared to existing chemical methods for producing graphene, this process requires less energy and gives a thinner and more stable material. Graphene having different physical and surface properties and different surface area thickness ratio could be produced since the reduction of functional oxide groups by using two different bacteria was provided differently and the capacity of each bacterium was different. Therefore, microbial reduction of graphene oxide appears to be a promising method for the development of new types of graphene-based materials and devices, avoiding the use of hazardous, environmentally friendly chemicals in a variety of types and applications, including nano-composites, conductive inks and biosensors.

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Abstract ID: 206

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Computational Electronic Materials

Keywords: Boundary Element Method, Three Temperature, Nonlinear Generalized Thermoelasticity, Functionally Graded Magnetic Thermoelectric Materials

A New Boundary Element Formulation and Analysis of Fractional-Order Three-Temperature Nonlinear Generalized Thermoelastic Problems of Functionally Graded Magnetic Thermoelectric materials

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The main aim of this article is to introduce a new fractional-order theory to contribute for increasing development of technological and industrial applications of functionally graded magnetic thermoelectric materials. This theory, called three-temperature nonlinear generalized thermoelasticity of functionally graded magnetic thermoelectric materials (FGMTM). In order to guide the current research field to the development of new functionally graded materials (FGM), we should successfully implement the computerized numerical methods that are used to solve and simulate difficult nonlinear FGM problems. The governing equations of the proposed theory are very complex to solve experimentally or analytically because of very strong nonlinearity. To overcome this, we need to develop new numerical techniques for solving such equations. Therefore, we propose a new boundary element method (BEM) formulation for solving the theory's governing equations. Due to the advantages of the BEM solution such as treating problems with complex shapes that are difficult to treat with traditional methods and does not require the discretization of the internal domain. Also, it requires low CPU usage and low memory storage. Therefore, the BEM is suitable for treating a wide range of advanced FGMTM applications. The numerical results are presented highlighting the effects of the effects of magnetic field and graded parameter on the thermal stresses in FGMTM. The numerical results also confirm the validity and accuracy of the proposed formulation and solution technique.

Abstract ID: 207

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Carbon/Carbon Composites

Keywords: Graphene, Electrochemistry, Laser writing, biopolymers

Three-dimensional (3D) graphene-like electrodes obtained by direct laser writing methods for electrochemical sensing

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The development of three-dimensional (3D) porous graphitic structures is of great interest for electrochemical sensing applications as such structures they can support fast charge transfer and mass transport through their extended, large surface area networks. In this work we present the facile fabrication of conductive and porous graphitic electrodes by direct laser writing techniques. Irradiation of commercial polyimide sheets (Kapton tape) was performed with a low cost laser engraving machine with visible excitation wavelength (450 nm), leading to formation of 3D Laser Induced Graphene (LIG) structures. The porous morphology of the composite material was assessed by electron microscopy; its graphene-like nature was characterized by Raman spectroscopy. Electrochemical characterization performed with inner and outer sphere redox mediators showed fast electron transfer rates, comparable to previously reported 2D/3D graphene-based materials and other graphitic carbon electrodes. Practical applications in the detection of ascorbic acid, uric acid, dopamine and mixtures of the above were demonstrated. Specifically, speciation of the three species was obtained without any need of surface modification. In addition, novel electrochemical sensors were fabricated by direct laser writing techniques on compostable biopolymers. Such composites showed fast scan rates and could be electrochemically measured for 25 minutes before showing signs of instability. After measurements residual electrodes could be dissolved in water in 1 hour. This work opens the way to the facile fabrication of low-cost, disposable electrochemical sensor platforms for decentralized assays.

Abstract ID: 208

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Theory of graphene, Mxenes and other two-dimensional materials

Keywords: 2D transition metal dichalcogenides materials, DFT, valleytronics, spin-orbit coupling

Cr substitutional doping and vacancy clustering as route to valley polarization in monolayer MoSe2 and WSe2

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The recent discovery of two-dimensional (2D) materials1 have provided a way to overcome development and standardization difficulties and new research area for nano-materials science and technology. 2D materials have revealed large potential for the new generation low-dimensional transistors, photo-emitting devices and spintronics due to their distinct crystal structures and electronic properties2, 3. Among the various field, valleytronics is considered to be a more recent area that depends on charges with a dispersion relation identified by two or more valleys with equal energy at different momenta4. Moreover, valley and spin control can open the possibility to valleytronic and spintronics in the same material5. In consideration of the obvious importance these properties, it can be interesting to investigate the questions of valley polarization as the spin and valley degrees of freedom are interlinked in 2D transition metal dichalcogenides based on selenium. Considering the interest in Cr-doped MoSe2 and WSe2 monolayers for spintronic and valleytronics applications, together with the lack of sufficient knowledge of their properties, we have explored the electronic and magnetic properties of MoSe2 and WSe2 monolayers by interplay between Cr doping at the Mo site and vacancy clustering. Our calculations are carried out within the framework of the spin-density functional theory with spin-orbit coupling. The incorporation of Cr into MoSe2 and WSe2 (as Cr is isoelectronic to Mo) can offer the possibility of electronic structure manipulation in monolayers semiconductors for applications in valleytronics

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Abstract ID: 209
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Bio-composites
Keywords: Low-density Polyethylene, Facilitated oxidation and subsequent biodegradation, Biobased pro-oxidant additives, Ultimate biodegradability and bio-recycling. Post bio-degradation.

Investigated triggered oxidation and subsequent bio-degradation of LDPE films composed with bio-based pro-oxidant additives for single-use commercial waste management applications.

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Low-density polyethylene (LDPE) films were melt extruded and blown moulded into two LDPE formulations 1% and 3% (w/w) labelled as (LDPE-1% and LDPE-3%). The formulated LDPE films were exposed to varying degradative (abiotic and biotic) conditions to investigate chemical oxidation and oxidation rate under photo-oxidizing conditions (natural sunlight) followed by bio-oxidation degradation to investigate potential biodegradability of the photo- and thermally oxidized test materials in simulated marine water, soil and compost environments for 180+ days. This investigation was focused on the introduction of functional groups in the LDPE polymer chain using the bio-based pro-oxidants. To monitor and determine oxidation degradation and oxidation rate thereof, different techniques were used. According to the FT-IR results, test samples exposed to photo- and thermal oxidation underwent chemical transformation, this was evident by development of new peaks which symbolized development of new functional groups in the carbonyl region. Carbonyl index increased with time as number of exposure days increased. According to GC-MS analyses, these carbonyl compounds detected were ketones, anionic acids, alcohols, carboxylic acids and aldehydes together with a series of short chain alkenes and alkanes. The photo- and thermally oxidized LDPE samples were observed to undergo molecular weight and molecular weight distribution decrease from GPC analyses. Oxidized LDPE-1% decreased from 404K Mw to 111K Mw after 200 days of photo-oxidation exposure whilst Oxidized LDPE-3% reduced from 293K Mw to 22K Mw after 100 days. Due to better responsive oxidation behavior, LDPE-3% was further investigated for potential biodegradability in soil, compost and simulated marine water. Biodegradation results of photo-oxidized LDPE-3% revealed mineralization to micro-organism activity observed as a 10.4% (181 days) biodegradation percentage in simulated marine water, a 20% (233 days) in soil, and a 52.6% (263 days) in composting medium. Oxidized LDPE-3% of low molecular weight properties showed to undergo active biodegradation by means of active microorganism with secondary products such as carbon dioxide (CO2), water (H2O) and new cell biomass. These results proved that LDPE films composed with biobased pro-oxidant additives can undergo photo- and thermal oxidation leading to material disintegration and fragmentation followed by subsequent bio-degradation leading to biological recycling of conventional LDPE films used for

single use commercial and ecological applications. After 180+ days of bio-degradation investigations, oxidized and bio-degraded films were retrieved and further analysed with TGA, DSC, SEM, FT-IR and GPC for post bio-degradation insights in material bio-assimilation.

Abstract ID: 210
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Polymeric composites
Keywords: Epoxy based composites, glass beads microparticles, alumina nanoparticles, weathering test, flexural strength, abrasion resistance

Investigation of Flexural Strength and Abrasion Resistance Improvement by Using Micron Size Glass Beads and Alumina Nanoparticles Reinforcement of Epoxy Matrix

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Investigation of Flexural Strength and Abrasion Resistance Improvement by Using Micron Size Glass Beads and Alumina Nanoparticles Reinforcement of Epoxy Matrix

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Epoxy based composite materials are widely used in many fields including aerospace, automotive industry and marine applications due to their good mechanical properties and low weight. The current research is investigating the effects of using glass beads micron size particles (9-13 micrometer) or alumina nanometer size particles (50 nm) as epoxy matrix reinforcements on the mechanical properties. Samples were produces using 0, 5, 10 and 15 % glass beads or similar percentages alumina nanoparticles that were well dispersed in the epoxy matrix. The degree of dispersion was evaluated using the Scanning Electron Microscopy (SEM). Some of the samples were then exposed to standardized accelerated weathering tests (cycles of UV radiation, high temperature and moisture) using a Q-Lab QUV equipment. The effects of the glass beads and alumina nanoparticles epoxy embedment was explored by conducting standardized flexural tests (Mark-10 tensile testing equipment) and abrasion tests (Taber abrasion tester equipment). Similar tests were performed on samples exposed to harsh environmental conditions. Different models were developed to theoretically describe the mechanical behavior of the epoxy composites. It was observed that flexural strength performance was not enhanced by the introduction of glass beads or alumina nanoparticles. However, the abrasion resistance was improved by using both materials with higher improvement observed in the case of alumina nanoparticles.

Keywords: Epoxy based composites, glass beads microparticles, alumina nanoparticles, weathering test, flexural strength, abrasion resistance

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Abstract ID: 211

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nano-Magnetic, Magnetic Memory and Spintronic Materials

Keywords: Polarized neutron reflectometry, Perpendicular magnetic anisotropy

Magnetic properties and SOT application for a W based PMA thin films

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Perpendicular magnetic anisotropy (PMA) in the CoFeB/MgO stack is currently under intense study, due to its advantages in providing low critical current for magnetic switching in the spin-orbital torque (SOT) devices. To obtain high magnitude of SOT, a number of heavy metals with spin-orbit coupling were studied, such as Pt, Ta, and W, among which W was reported to have the largest spin hall angle. Meanwhile, the commercialization of such structures requires PMA to be compatible with COMS integrated circuits, which generally can endure the annealing above 450℃. Here, we reported that the PMA in W/Zr/CoFeB/MgO is found to be robust up to 450℃. The origin of PMA is investigated by using polarized neutron reflectometry (PNR)1, which enables us to discuss the role of boron in the formation of PMA by inserting a thin Zr film. The PNR measurement was carried out at the multi-purpose reflectometer (MR) at China spallation neutron source2, which is an instrument optimized for examining thin films with nanometer scale structure, especially in regard to their magnetic properties.

Moreover, the Hall bar of W/Zr/CoFeB/MgO were also patterned. The current for magnetic switching behavior via the spin-orbital torque will be discussed.

Abstract ID: 212

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Non-destructive Inspection Techniques for Composite Materials and Structures

Keywords: Piezoelectric, interface debonding detection, multiscale simulation, mesoscale structure of concrete core, stress wave, aggregate distribution, aggregate shapes

Multiscale simulation on the mechanism of debonding defect detection for concrete-filled steel tubes with piezoelectric materials

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Interface debonding between concrete and steel tube of concrete-filled steel tubes (CFSTs) leads to negative effects on their mechanical behavior and piezoelectric-lead-zirconate-titanate (PZT) has been employed as actuator and sensor to detect the interface debonding defect. In traditional structural analysis, concrete has been assumed to a homogenous materials even though concrete is a typical multiple composite comprised of coarse and fine aggregates, mortar matrix, interface transition zones (ITZs) and pores, as well as initial defects. The mesoscale structure of concrete might has an influence on the wave propagation in CFST structures. Therefore, it is necessary to further study the mechanism of the wave measurement based interface debonding detection approach considering the influence of mesoscale structure of concrete on the stress wave propagation and the response of PZT sensor embedded in concrete core or bonded on the surface of the CFST. In this paper, mesoscale numerical concrete models including circle, ellipse and irregular polygon aggregates with different distribution are employed to model concrete core of CFST and wave propagation and the response of embedded and surface mounted PZT sensor of rectangular CFST members are simulated. The effect of randomness and heterogeneity in aggregate distribution and aggregate shapes are discussed. The stress wave propagation in the cross-section of the rectangular CFST members without and with interface debonding defects under sweep frequency excitation are simulated. The sensitivity of a defined damage index based on wavelet packet energy spectrum on the sensor response is investigated in details. The results show that the mesoscale structures of concrete core has a limited influence on the PZT sensor measurement when compared with it of interface debonding defects. The results show the feasibility of the wave measurement based interface debonding defect detection approach for CFST members even the mesoscale structure of concrete core is considered.

Abstract ID: 213

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Industrial applications of composite materials

Keywords: p-i-n diode, a-IGZO, thermal sensor

Built-in-Hole a-IGZO p-i-n Diode for Chip-Scale Temperature Mapping

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In this paper, we report design, fabrication and characterization of a vertical built-in-hole p-i-n diode structure using amorphous indium gallium zinc oxide (a-IGZO). The ultimate goal of this design is to use the in-hole a-IGZO p-i-n diode as an accurate on-chip temperature sensor for integrated circuit chips. Since the built-in-hole a-IGZO sensor can be placed right underneath each MOSFET on a chip, it will allow real-time whole-chip temperature mapping with ultra-fine spatial resolution down to transistor level. This novel design opens a door for accurate full-chip thermal management in real time. In this work, a CMOS-compatible process module was developed to fabricate a a-IGZO diode consisting of the following process steps: etching a 10μm deep hole inside a silicon substrate, p-doping in the deep hole to form the pregion, depositing a 10nm aluminum film as the i-layer by atomic layer deposition (ALD), and sputtering to deposit a 150nm a-IGZO layer as the n-region. A a-IGZO p-i-n diode is then formed in the deep hole in the Si substrate. The process module was developed for room temperature to <200℃, hence be compatible to the CMOS back end of line (BEOL) process. DC sweeping test from 0V to 15V across a wide temperature range was conducted for the fabricated a-IGZO p-i-n diode to evaluate its I-V-T behaviors for temperature sensing application. Fig. 1 shows clearly that the built-in-hole a-IGZO p-i-n diode works well and is sensitive to temperature variation. Therefore, the designed built-in-hole a-IGZO p-i-n diode can be used as a temperature sensor to generate real-time full-chip temperature map for power

and thermal management of IC chips.

Abstract ID: 214

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster/Oral Presentation

Topics: Artificial photosynthesis

Keywords: Bioinspired, carbon nitride, NADH regeneration, photocatalytic

Bioinspired Photocatalytic NADH Regeneration by Graphitic Carbon Nitride based Materials for In-situ Coupled Enzymatic Catalysis

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In natural photosynthesis, following light harvesting by chlorophyll molecules, photoinduced electrons are passed through electron transport chain to the enzyme ferredoxin-NADP reductase, leading to the reduction of nicotinamide adenine dinucleotide phosphate (NAD(P) to NAD(P)H), completing the storage of light energy in one kind of “energy currency” of the cells. Inspired by the photosynthesis, graphitic carbon nitride was employed by us for NADH regeneration in the presence of [Cp*Rh(bpy)Cl]Cl as an electron and proton mediator. By engineering the graphitic carbon nitride into various nanoarchitectures including diatom-inspired nanostructures, in-situ synthesized film electrode and single-atom coupled system, the high NADH regeneration efficiency driven by visible light could be accomplished. Therefore, the in situ NADH regeneration rate is high enough to reverse the biological pathway of the three consecutive dehydrogenase enzymes (formate dehydrogenase, formaldehyde dehydrogenase, and alcohol dehydrogenase, respectively), which allows for instance the successive conversion of formaldehyde to methanol and the reduction of carbon dioxide into methanol and other enzymatic reactions.

Abstract ID: 215

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Solar Cells

Keywords: Photon Up-conversion, Dye-sensitized Solar Cell, Harvesting Infrared Radiation, Proof of Concept

Harvesting Up-converted Infrared Radiation for Dye-sensitized Solar Cells to Perform in the Dark

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Solar spectrum incident on the Earth surface consists mainly of 5% ultraviolet, 40-45% visible and 50-55% infrared radiation. However, dye-sensitized solar cells (DSCs) only utilize UV and some visible components but not the major IR fraction since IR is incapable of electronic excitation. In order to utilize IR radiation, these IR photons have to be added to get UV or visible radiation via the process known as photon up-conversion. Photon up-converting crystals based on NaYF4 doped with Er(III) or Yb(III) and both Er(III) and Yb(III) are used in bio-imaging since IR radiation has deeper penetration when compared to that of UV and visible and the detection is from colors generated in the visible range. For the first time, these up-converting lanthanide crystals were used together with N-719 dye to coat interconnected nanoparticles of TiO2 with them to be used in both liquid electrolyte (I-/I3- in acetonitrile)-based and in all DSCs. The presence of lanthanide crystals on TiO2 particles is proven by XRF measurements and its ability to absorb in near IR by UV-visible-NIR spectroscopy. Although liquid-type DSCs did not perform with infrared illumination in the dark, the all solid-state solar cell gives appreciable efficiency of 4.5% with 1 Sun illumination (UV-Visible-NIR) and 0.4% efficiency only with NIR illumination, in the dark, despite the fact that the intensity of NIR source used is much less than 1 Sun. The performance of the liquid electrolyte-based DSC is inferior to one without up-conversion crystals even with 1 Sun illumination and it did not give any efficiency with infrared illumination alone. This is mainly due to evaporation of the volatile solvent and consequent drying up of the DSC. A 4.5% efficiency for a all solid-state DSC is perhaps the highest so far recorded. The fact that it works only with IR radiation indicates that solar cells can be fabricated to work even in the night. This is an entirely new concept and this research gives evidence for the proof of concept.

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Abstract ID: 216

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Nanogenerators and self-powered nanosystems

Keywords: Carbon Nanotube, Yarn, Energy Harvester, Emergency

Harvesting electrical energy of carbon nanotube yarn in sea water for self-powered devices

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Mechanical energy harvesters are needed for such diverse applications as self-powered wireless sensors, structural and human health monitoring systems, and cheaply harvesting energy from ocean waves. We report carbon nanotube yarn harvesters that electrochemically convert tensile or torsional mechanical energy into electrical energy. The carbon nanotube yarn is lightweight, mechanically-robust and non-corrosive to be suitable for long time use in electrolytes including sea water. Fundamentally, these yarns are supercapacitors. In a normal capacitor, you use energy – like from a battery – to add charges to the capacitor. But in our case, when you insert the carbon nanotube yarn into an electrolyte bath, the yarns are charged by the electrolyte itself. No external battery is needed. When a harvester yarn is twisted or stretched, the volume of the carbon nanotube yarn decreases, bringing the electric charges on the yarn closer together and increasing their energy. This increases the voltage associated with the charge stored in the yarn, enabling the harvesting of electricity. Stretching the yarns 30 times a second generated 250 watts per kilogram of peak electrical power, when normalized to the harvester's weight. Our self-powered emergency signal device is based on the carbon nanotube yarn and technology as mentioned above. The product consists of a balloon part that floats the human body by buoyancy in the sea and a harvesting part that is connected with it and generates electricity by the swirling of sea water. The special thing about our products is in the harvesting parts. The carbon nanotube yarns harvest the mechanical energy of the ocean to produce electricity, store and boost electrical energy in the connected circuitry to drive electronic equipment like LED. Generated electricity could drive LED and air balloon like life jacket and it can increase the probability of survival in ocean emergency. The device harvests the mechanical energy from the movement of sea water and use it as electrical energy, so it has the advantage of being semi-permanent and safer. It can be used in all types of existing life-saving equipment such as marine leisure sports including surfing, navy, passenger ships and airplanes.

Abstract ID: 217

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Nanogenerators and self-powered nanosystems

Keywords: Particulate Matter, Nano Sensor, Air Quality, Self-powered, Energy Harvesting

A Non-optical Air Quality Sensor driven by Energy Harvester

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High concentration of particulate matter (PM) 10 and 2.5 has arisen with frequency in South Korea. PM is known for having adverse effects on the health such as bronchus, asthma and conjunctivitis etc. It is important to monitor the air environment in real-time. As a possible solution, air quality sensor can be employed for air-quality monitoring system. Almost the air quality sensors, meanwhile, are composed of batteries and sensing parts. Sensing part operates using a gravimetric, light scattering and beta gauge method. However, it is difficult to maintain and analyze to the general public and it is needed to connect the power line or rechargeable batteries for the power source of sensors. In this study, it is to make an air quality sensor that is composed of organic materials and is applying a non-optical detection method. The air quality sensors are fabricated by micro-electromechanical systems (MEMS) technique. Based on a PVDF-TrFE and PTFE films, triboelectric nanogenerator (TENG) is employed for power supply in air-quality sensor. It uses the simplest design as a contact-separation mode. The TENG and sensor are combined with a copper wire and construct on a one substrate.

Abstract ID: 218

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Ferrites and Garnets

Keywords: Spinel ferrite, EM-absorption, Permeability, Permittivity, Reflection Loss

Gigahertz range EM absorbing property of Ni-Zn ferrites powder-epoxy composites

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Cubic-structured Ni–Zn spinel ferrites are some of the important magnetic ceramics used in various electromagnetic devices, such as telecommunication systems, microwave devices, and power transformers because of their high magnetic permeability with a small magnetic loss and high electrical resistivity [1-3]. Their applications in high-frequency devices can be classified based on the real (μ') and imaginary (μ") parts of the complex permeability, μ = μ'- jμ". A high μ' and very low tan δμ = μ" / μ' are required for applications in magnetic field shielding, wireless charging, inductors, and transformers. In addition, a large μ" is required for the electromagnetic wave (EM) absorber employed in the corresponding frequency range.

In this study, spinel ferrites NixZn1-xFe2O4 (x=0.4, 0.5, 0.6) were prepared by sol-gel method. X-ray diffraction (XRD) analysis confirmed that crystalline single spinel phase could be formed after annealing the sol-gel processed powders at T ≥ 400°C. Scanning electron microscope (SEM) was used for the study of microstructure. The grain size of these sample are in range of 100 ~ 500 nm. The Ni-Zn powder-epoxy(10wt%) composite samples in form of toroidal ring were fabricated for the complex permittivity and permeability measurements. Using the μ = μ' - jμ″ and ε = ε' - jε″, measured by vector network analyzer (1MHz ≤ f ≤ 18 GHz), the reflection loss (RL), which reflect the EM wave absorbing performance, were calculated [4]. The RL map as functions of absorber thickness (d) and frequency (f) also plotted. Each composite sample of x=0.4, 0.5, 0.6 showed two major RL peaks where intensive EM absorbing occurs. The first RL peaks (RL < -40 dB) were found in the f of 2~3 GHz range at d in 5~8 mm, while the second RL peaks (RL<-30) were in the 8~13 GHz at 3~4 mm. These results show that the Ni-Zn ferrite-resin composite are very promising materials for EM wave absorber applications. Details on the effects of composition x and sample processing conditions on the EM absorption properties will be discussed.

Abstract ID: 219

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster/Oral Presentation

Topics: Photocatalytic and electrochemical water splitting
Keywords: Hematite, spin coating, Spectroelectrochemistry, photocathode, water splitting

Transforming α-Fe2O3 Into Photocathode For Solar H2 generation Through Band Gap Engineering By Codoping It With Zn and Cu

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Intense research on alternative energies has been going on globally to find a solution to overcome energy crisis. Harvesting solar energy is a good choice among the naturally abundant energies. Hydrogen production by solar water splitting (SWS) is considered as a promising approach for storing solar energy. Hematite (α-Fe2O3) is an attractive material as photoelectrode in SWS due to its ban-gap (Eg = 2.2 eV), lying nearly in the optimum range for SWS. This band-gap allows absorption of solar energy in the visible region, where the sun emits maximum energy. Besides, a-Fe2O¬3 is naturally abundant in the earth's crust and is therefore, a low-cost material. It is also corrosion-resistant in acidic and alkaline medium [5-10]. But α-Fe2O3 cannot be used as photocathode that produces H2 in solar water splitting because of its conduction band edge position. This report presents an approach to engineer the band edge position of Fe2O3 by codoping Fe2O3 with Zn and Cu that resulted a shift of conduction band edge position of Fe2O3 above the H+/H2 reduction potential enabling it to be used as photocathode. Fe2O3 thin film codoped with Zn and Cu was synthesized by a simple one-pot synthesis route. After confirming the chemical structure, crystal structure and the surface morphology of pristine and codoped Fe2O3 the band energies of codoped Fe2O3 were investigated by UV-Vis spectrophotometry and spectroelectrochemistry (SEC). At 1.5% Zn and 0.5% Cu doping the conduction band minima was found to be at -0.8 V vs normal Hydrogen Electrode (NHE), which was above the H+/H2 reduction potential. Finally, under 1.5 AM simulated sunlight Zn and Cu codoped Fe2O3 was found to split the water indicating its possible use as a photocathode.

Abstract ID: 220

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Electrical, optical, electrochemical, thermal and mechanical properties of graphene, Mxenes and other two-dimensional materials

Keywords: Dichalcogenides, Molybdenum disulfide, Au nanorod, Photothermal therapy

Two –dimensional MoS2 Nanosheets Decorated by Gold Nanorods for Photothermal Theraphy

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MoS2 is one of the two-dimensional (2D) transition metals dichalcogenides that has been found its application in fields of biomedical such as tumor photothermal therapy and drug delivery due to its high near-infrared (NIR) absorption ability and unique two-dimensional (2D) structure with large surface area. In this work, molybdenum disulfide nanoflakes (MoS2) were synthesized by hydrothermal method in presence of polyethylene glycol (PEG). PEG modifies MoS2 surface therefore this sample has a good stability in biomedicine solutions and water. Au nanorods have shown to exhibit high therapeutic properties as hyperthermal agents since the local temperature around the Au nanorod can be increased by laser illumination because of the tunable Au nanorod surface plasmon bands in the NIR region. Au naorods have photothermal properties at ~808 nm beacase it exhibits localized surface plasmon resonance. Therefore decorating MoS2 by Au nanorods (Au−MoS2) has increased MoS2 photothermal properties. Both samples (MoS2 and Au−MoS2 hybrids) were analyzed by XRD, TEM, UV-visible spectrometer, Raman, AFM, FTIR, photothermal therapy. TEM images show 2D layer structure (2-3 layers) with high porous network with Au nanorods which interplace on MoS2 nanoflakes surface. The photothermal effect of solutions of the samples was investigated in a range of concentrations and irradiation with a continuous wave laser at λ = 808 nm. This search offers a promising route to enhance the photothermal heat of MoS2 nanoflakes and provides suggestive insights for developing high-performance materials in photothermal therapy and can be used in MRI as well.

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Abstract ID: 221

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: Photon Up-conversion, Catalysts for Water Photo-splitting, Harvesting Infrared Radiation

Water Photo-splitting for Hydrogen Generation using transition Metal Ion-or Lanthanide Ion-Doped Titanium dioxide Nanoparticle based Photon Up-conversion Materials

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Hydrogen is the cleanest and greenest fuel that can be used directly in internal combustion engine of motor vehicles and in fuel cells for cleaner and greener energy generation. However, hydrogen as hydrogen (H2) molecules do not exist in the atmosphere. H2 is abundant in the bound molecular forms: mainly as water and hydrocarbons. H2 is mainly produced by petroleum cracking and the generated gas is used mainly onsite for production of petroleum-based chemicals and also for ammonia synthesis. H2 is also produced by water electrolysis though the cost of production depends on cost of electricity. Honda and Fujishima first discovered photo-assisted electrochemical water splitting to H2 and O2, in 1972, using illuminated titanium dioxide electrodes. However, being a large band-gap semiconductor, TiO2 absorbs in the UV region below 380 nm which is only present as 5% in the incident solar spectrum. Extensive research carried out since then enabled the development of efficient electron-hole separation to suppress their recombination. Deposition of noble metal (Pt or Pd) islands to catalyze H+ reduction and RuO2 for hole capture for water oxidation are one such important strategies introduced. However, these catalysts lack the capability for utilization of full solar spectrum. In this research, novel strategy was developed where silver islands were deposited on TiO2 nanoparticles for some visible light harvesting through their surface plasmon resonance effect and infrared upconverting electronic energy levels were introduced by doping TiO2 with selected transition and lanthanide metal ions. A range of catalysts without and with Ag Islands [Ir(IV)-TiO2, Eu(III)-TiO2, Ho(III)- TiO2, Nb(V)-TiO2, Sm(III)- TiO2, Ir(IV)-TiO2, Cu(II)-TiO2, Ir(IV)-TiO2-Ag, Eu(III)-TiO2-Ag, Ho(III)- TiO2-Ag, Nb(V)-TiO2-Ag, Sm(III)- TiO2-Ag, Ir(IV)-TiO2-Ag and Cu(II)-TiO2-Ag] were synthesized and their infrared absorption verified by UV-Visible-NIR spectroscopy. Materials were duly characterized by powder XRD, XRF, FT-IR and SEM techniques. All these catalysts were shown to be more efficient in water photo-splitting when compared to that with bare TiO2 and TiO2 with only Ag Islands. However, in the absence of sacrificial hole-scavengers hydrogen and oxygen gases produced recombined generating excess heat that damaged the crystal lattice of the catalysts. Besides, when a gas mixture is generated its separation needs additional effort. As such, methanol and ethanol were used as sacrificial hole-scavengers to prevent oxygen generation. These catalysts generated hydrogen gas continuously when kept exposed to sunlight, in the stray light in the lab and also with upconverted infrared radiation when kept in the dark in the ambient laboratory conditions. Among these systems, Cu(II)-TiO2-Ag, Nb(V)-TiO2-Ag and Ir(IV)-TiO2-Ag had the best performance of generating over 250 µl of H2 gas per hour.

Abstract ID: 222

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Magnetism and Magnetic Materials

Keywords: magnetic impregnation, magnetization, Fe K-edge analysis, oxidation state, ferromagnetic ordering

Magnetic impregnation on K0.5Na0.5NbO3 through multiferroic doping

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The (K0.5Na0.5)NbO3 composition was prepared through solid state reaction, while doping material BiFeO3 through sol-gel self-combustion method. The magnetic impregnation occurred in conjunction with dopant dissolve into the matrix, the method adopts standard procedure of ceramic processing, calcination at 5750C for 6 hours then sintering at 1100ºC for 2 hours. The characterization includes X-ray diffraction (XRD), X-ray spectroscopy (XAS), and superconducting quantum interference device (SQUID) magnetometer. Crystal structure of the studied material was tetragonal at room temperature. XANES Fe K-edge analysis revealed that the absorption energies consist of quadrupole transition 1s → 3d (t2g and eg) and dipole transition 1s → 4p (pπ and pσ). These energies were higher than that of Fe2O3 suggesting the oxidation state of Fe was a mixture of 3+ and 4+, thereby creating defects in the structure 〖Fe〗_Nb^", 〖Fe〗_Nb^'and influencing magnetization. The paramagnetic (K0.5Na0.5)NbO3 become para-ferromagnetic after dopant BiFeO3 dissolved in the matrix. It is believed that the origin of magnetic moment is 3d unpair electrons of Fe occupied in octahedron BO6 and influenced by the existence of ferromagnetic ordering interaction Fe3+-O2--Fe4+ of side by side octahedron.

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Abstract ID: 223

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Solar Cells

Keywords: TiO2, crystallization, carrier selective, atomic layer deposition

The crystallization of TiO2 grown by atomic layer deposition as the thickness and annealing condition change

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TiO2 has been used in many branches, such as photocatalyst, water splitting, photoanode in dye-sensitized solar cells. Recently, TiO2 begins to be paid attention in Si solar cell as the passivation layer and the electron selective contact layer. Highly B- or P-doped regions of deposited amorphous or polycrystalline silicon need to extract electrons and holes, respectively. But the doped regions exhibit high recombination and/or parasitic absorption losses, posing a fundamental limit to device performance. This has accelerated a research focused on the search for carrier selective materials that can reduce the losses at the c-Si solar cell contacts, including transition metal oxides, organic polymers and alkali metal salts. Thin TiO2 layer was grown by atomic layer deposition and its crystallization was analyzed by XRD and TEM. In this study, we deposited TiO2 layer by using TDMAT(Tetrakis Dimethyl Amido Titanium) and TTIP(titanium tetra-isopropoxide [Ti(OCH(CH3)2)4, TTIP] precursors and H2O oxidant. and studied the crystallization factors of TiO2 thin films to form electron-selective contacts on c-Si solar cells, such as the thickness and annealing condition. We also studied how TiO2 crystallization influences the bandgap, passivation and electron selective characteristics.

Abstract ID: 224
Symposium 4: Functional Composite Materials (FCM)
Poster/Oral Presentation
Topics: Multifunctional composites
Keywords: Phonon modes, Elastic Properties, Bulk Metallic Glass, Pseudopotential

Phonon Dispersion Curve and Elastic Properties of Pr55Al10Ni10Cu1-xFex Bulk Metallic Glasses

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The present paper deals with the theoretical study of phonon modes and elastic properties of Pr55Al10Ni10Cu1-xFex bulk metallic glasses. The Hubbard-Beeby approach connotation with our well define local model potential has been applied to compute the collective modes for present alloys. Four different local field correlation functions of Hartree (H), Taylor (T) , Farid et al (F) and Sarkar et al (s) are employed to find the influence of the screening effects on the vibrational modes of Pr55Al10Ni10Cu1-xFex bulk metallic glasses. The computed phonon dispersion curves show all broad features of the collective excitation. It observed that out of three local field correction function, Hartree screening function gives the good agreement with experimental data compared to other three screening functions. It can be concluded that the selection of local field correlation functions plays an important role in the determining elastic properties of disorder system. Also, present model potential is able to explain the collective excitation of bulk metallic glasses.

Abstract ID: 225

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Dielectric, Ferroelectric and Piezoelectric materials

Keywords: Composite materials, Dielectric characteristics, Maxwell-Garnett model, Microwaves

Composite laminate materials with low dielectric loss: theoretical model and dielectric characterization

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Organic matrix composite materials have a dominant position in the transport sector. These materials, mainly made of reinforcement fibers impregnated by a thermosetting resin, allow the fabrication of lightweight and mechanically resistant structural panels. Moreover they promote embedded electronic applications. With a societal and technological evolution ever more connected, the integration of antennas within load-bearing composite panels is a major area of interest. A few works have developed this original approach. Manac'h and al. [1] demonstrated similar microwave performance between a pure composite laminate antenna and a copper antenna in the 600 MHz – 2.1 GHz frequency band. Other antennas have been made from sandwich composite panels directly embedded within vehicle structures [2]. The present work aims to theoretically and experimentally study various dielectric composite laminate panels that may be used as support (substrate) and/or radome of antennas operating at microwaves. Composite laminate materials have been manufactured with E-glass, S2-glass and quartz fibers, impregnated with polyester, epoxy and urethane acrylate type resins by the standard vacuum infusion process. The two-dimensional Maxwell-Garnett's law [3] has been developed to theoretically retrieve the dielectric characteristics (permittivity εr and loss tangent tgδ) of the above composite laminate materials at 1 GHz. The experimental study of the composite materials has then been carried out over two frequency bands through impedance measurement (100 MHz – 1 GHz) and free space method (18 GHz – 26 GHz). Dielectric permittivities ranging from 3.0 to 4.3, and loss tangents from 3×10^-3 to 1.3×10^-2 have been measured. Experimental results are compared with those retrieved from the theoretical model. A strong fit on εr and tgδ values is achieved, demonstrating the relevance of the 2D Maxwell-Garnett model. Moreover a permittivity εr = 3.1 and a loss tangent tgδ = 3×10^-3 at 1 GHz, and (εr = 3.2; tgδ = 6.5×10^-3) at 22 GHz have been achieved with the quartz fibers/urethane acrylate type resin composite laminate material. Therefore, the use of this composite laminate for low loss load-bearing composite panel applications at microwaves becomes totally relevant.

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Abstract ID: 226

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Nanocomposites

Keywords: Graphene, CNT, PANI, Supercapacitor

PANI-CNT-GO nanocomposites architecture for supercapacitors

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An ultra-high dielectric constant nanocomposites architecture of Polyaniline (PANI) - Carbon Nanotube (CNT) – Graphene oxide (GO) was prepared by using polymerization of aniline in an aqueous dispersion of CNTs in the presence of grapheme oxide (GO). 5 mg of CNTs was dissolved in H2SO4: HNO3 (2:1) and total solution was 25 ml. After that, solution was sonicated for 24 hours in order to disperse CNTs bundles. The GO is able to attach with polymer chain and with CNT due to presence of lots of epoxide, hydroxyl and carboxyl groups at the edge and its surface sites. The thin film of hybrid nanocomposites was characterized by using SEM, FTIR and X-Ray diffraction (XRD) techniques. The dielectric constant, dielectric loss and A C conductivity of the nanocomposites were studied as a function of temperature and frequency. The decrease of dielectric constant with frequency has been observed. The high dielectric constants have been observed at 600C due to increase of charge carriers through the hoping mechanism. The each matrix of PANI-CNT-GO will act as a tiny supercapacitor. The influence of large number of tiny supercapacitors will influence the resultant energy storage capacity. It is assumed that the resultant energy is attributed by algebraic sum of energy due to tiny supercapacitors.

Abstract ID: 227

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Magnetism and Magnetic Materials

Keywords: Spin Orbit Coupling, Strain Disorder, Epitaxial Thin Films, Spectroscopy, Magnetism

Spin-Orbit Coupling Escorted through Strain Diversity

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Intentionally, we have successfully grown strain disordered epitaxial thin films of itinerant ferromagnet SrRuO3 (SRO) on different substrates which are relaxed in nature. Length scale-dependent strain (strain diversity) is responsible to enhance magnetic moment in these films, while the films possess a low spin state that is confirmed by soft x-ray absorption spectroscopic study. We observed charge transfer phenomena during the investigation of chemical state using X-ray Photo-electron spectroscopic study which is a result of the presence of strong hybridization between metal ions and ligands. Resonance photo-electron spectroscopic study again confirmed strong hybridization due to a large screening effect that resulting in a reduction in the core-hole interaction. Of particularly, the presence of strong hybridization and broaden nature of the metal ion band at the Fermi level lead an indication towards the presence of spin-orbit coupling. Thus, we have investigated this issue and found the presence of spin-orbit coupling. The resulted values were calculated using a relation of branching ratio at M3 and M2 absorption edges of Ru ion. In addition to that, X-ray magnetic circular dichroism measurement confirms the significant angular magnetic moment along with the spin magnetic moment in thin films. We have found a clue regarding the strong modification in octahedral rotation across the magnetic ordering using temperature-dependent Raman spectroscopic study. Therefore, we conclude that the strain diversity imposes to the octahedral rotation in a specific way in which the orbital quenching is diluted through the reduction in the strength of the sigma-bond and increase in the strength of the pi-bond. Our study offers a new insight regarding a critical length scale of strain disorder to stabilize the orbital de-quenching or strong spin-orbit coupling in 4d transition metal oxides which resulting in the enhanced magnetic moment and large coercivity. Now, a non-equilibrium phonon process (responsible for electron-phonon coupling in this system) and the stabilized strong spin-orbit coupling makes this material very promising for the functional applications like spintronics, optoelectronics etc. The presented pathway will open new doors for potential applications.

Abstract ID: 228

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multi-scale Modeling of Graphene- and Carbon Nanotube-Reinforced Composites

Keywords: Graphene nanopletelet, Glass Fiber, Moritanaka method

Micromechanical Modeming of Hybrid Glass Fiber Laminated Composites added with Graphene Nano Platelets

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The standard engineering materials are being fast replaced by composite materials due to their superior strength to weight ratio, ability to be custom tailored and their remarkable stiffness characteristics. Due to the above mentioned positive traits, these novel materials are finding their application in every wakes of life and are no more considered as a space age material. In the last decade, composites with nano particle infused matrix are a major research topic due to its potential to overcome the inherent weakness of laminated composite materials like weak intralaminar fracture toughness, tendency to delaminate etc. Among the different types of carbon based nano fillers, graphene is the most novel one. As such, the requirement for prediction of the properties of graphene based laminated composites has arisen. In the present study an attempt has been made to predict the stiffness matrix of the graphene nano platelet infused glass fiber reinforced laminated composites using micromechanical methods. Provision for accommodating the agglomeration and property variation of graphene is made in the program for calculating the stiffness. The mathematical modelling confirms that agglomeration of nano platelets drastically reduces the effective properties of GNP infused laminated composite. The proposed model also shows that a variation in the platelet size can cause significant variation in Young's Modulus and Poisson's Ratio. The weight fraction's under consideration in this study, i.e. .5% and 1% of GNP improves the tensile properties, inter laminar and intra laminar properties of glass fibre laminated composites. The addition of nano platelets increases the stiffness of the GNP infused laminates. A reduction in platelet size of graphene can give better results for laminated composites as the filtering effect of the glass fibre will be reduced and a more even distribution of graphene in the epoxy can be expected. The specimen cutting method and machine error might have caused the significant variation in the predicted and experimental results.

Abstract ID: 229

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Bio-composites

Keywords: The next generation of complex functional material evolution, Heterostructure orthogonal interaction, Model

Complex functional materials evoluted from heterostructure orthogonal interaction model

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Complex functional materials evoluted from heterostructure orthogonal interaction model

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The next generation of complex functional materials is rapidly transforming cross-disciplinary frontier field like quantum materials and their devices etc., which are solution-nanocrystals, leading to creating the core quantum unit of scalable qubit bits (qubits), therefore solving problems in computing, sensing or metrology, but a grand challenge in complex functional material science is to develop general methodologies for finding the right interaction model and corresponding theory1. Complex functional materials evoluted from heterostructure orthogonal interaction model approaches were herein postulated for beating the challenge, as demonstrated by author's issued patents in China and USA. A tetra-heterostructure orthogonal interaction model approach not only resulted in either a tetra-targeted therapy strategy for vital organs and vascular endothium growth factor of human cancer cells, but also generated bottom-up self-assembled conducting photoluminescence nanomedicine thin-films and crystals, quantized conductance junctions, bistable quantum wire arrays or redox quantum dot room temperature qubit networks, which paved a general way towards quantum computing, quantum sensing, quantum-level metrology model approaches for future applications. It is concluded that heterostructure orthogonal interaction model approaches to novel complex functional material evolution may offer a promising route to greatly enhance national security, economic impetus, Sino-USA even international society health, leading to satisfying un-met needs worldwide or beyond.

Key Words: The next generation of complex functional material evolution, Heterostructure orthogonal interaction, Model

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Abstract ID: 231

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Electromagnetism

Keywords: Hall effect, electrical resistance, asymmetric scattering coefficient

Determination of parameter of asymmetric electron scattering of conductivity of intermetallic compounds of Gd-In system

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In work [1] results of experimental data of coefficient of Hall of RH and residual specific resistance of □O of the intermetallic Gd-In connections are given in a wide interval of temperatures and concentration. As is known, in the paramagnetic region, the Hall coefficient RH is expressed by the following formula:

RH = RO + 4□□ RS , (1)

where, RO and RS is a normal and abnormal component of coefficient of Hall, □ is paramagnetic susceptibility. Asymmetric scattering is characterized by the difference between right and left scattering probabilities. Several rules make it easier to select members of the scattering probability that satisfy the Hall effect. Were investigated are connected, the containing various concentration of Gd and it turned out that asymmetric dispersion is proportional to the residual resistance of □O, that is concentration. In particular, at sufficiently high temperatures, RH can be approximated with the expression [2]:

RH= RO+a (□O / T), (2)

where, a - asymmetric scattering coefficient dispersion of electrons in rare-earth metals (REM), □O - residual specific resistance. From dependence of RH(□O/T), it is defined normal and abnormal parts of coefficient of Hall in the studied samples which are well correlated with dependence of RH(□). From dependence of RH(□O/T) values of coefficient of asymmetric dispersion of electrons of conductivity and in the studied samples are estimated. The calculations are given in Table. It can be seen from Table 1 that in the composition with increase of indium concentration, values of asymmetric electron scattering coefficient of conductivity of studied intermetallic compounds increase. This appears to be due to the presence of local orbital moments and hence some kind of orbital exchange between conduction electrons and localized electrons. That is, in the test compounds, the Gd component is present as impurities.

Asymmetric conductivity electron scattering coefficient values

№ Connections a, (K/Tl)

1. Gd3In5 0.55

2. GdIn3 1.10

As our calculations have shown, the results of the values of asymmetric scattering coefficient of conduction electrons, which for intermetallic compounds Gd-In in order of values, coincide with the results obtained by the authors of [3] for pure REM.

Key Words: Hall effect, electrical resistance, asymmetric scattering coefficient

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Abstract ID: 232

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Functional Magnetic Materials

Keywords: Magnetoelectric effect, Iron hydroxide, Goethite, Raman spectroscopy, Lattice dynamics calculations

Spin–Lattice Interaction in Magnetoelectric α–FeOOH

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Iron hydroxide alpha-FeOOH, known also as goethite, is among the most abundant iron bearing minerals in the Earth's crust. It has been known for decades as an antiferromagnetic insulator with a relatively high Neel temperature, TN = 120 deg C [1]. Recently, on the basis of predictive DFT+U and Monte-Carlo simulations, it has been hypothesized that α-FeOOH displays significant linear magnetoelectric effect below TN [2]. This fact revives the interest to this compound as a nonexpensive and environmentally friendly alternative to other magnetoelectric materials. So far, there is no direct experimental evidence for the suggested magnetoelectric coupling in alpha-FeOOH. Here we interpret the results of our recent Raman measurements on alpha-FeOOH, which reveal anomalous behavior of the lineshape and intensity of specific phonons near TN [3]. On the basis of supporting lattice dynamics calculations we identify the vibrations of the bridging oxygen atoms, which mediate the spin-lattice interaction in this compound. Our results shed light on the physical mechanism of magnetoelectric coupling in alpha-FeOOH.

Acknowledgments: This work was supported by the Bulgarian-Russian bilateral project KP–06–15/2019 funded by the Ministry of Education and Science of Bulgaria.

Key Words: Magnetoelectric effect, Iron hydroxide, Goethite, Raman spectroscopy, Lattice dynamics calculations

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Abstract ID: 233
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Nanocomposites
Keywords: Glassy carbon electrode, nanocomposite, platinum nanoparticle, jute carbon, nitride sensor

Enzymeless Electrochemical Detection of Hazardous Nitrite by Platinum Nanoparticle Coated Jute Carbon Modified Glassy Carbon Electrode

Md. Rabiul Hasan[1], Al-Nakib Chowdhury[1], A. J. Saleh Ahammad[2], Chanchal Kumar Roy[1], Md. Shakhawat Hossain Firoz[1], Md. Abdul Aziz[3]

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Aiming at constructing a new nonenzymatic electrochemical nitrite sensor, we have prepared a glassy carbon electrode modified with Pt nanoparticle (PtNPs) coated carboxylated activated jute carbon (PtNP_CAJC-GCE) synthesized from jute (Corchorus genus) sticks by using NaHCO3 as activating agent at 850 oC and subsequent functionalization by acid treatment. Surface morphology, and chemical composition of PtNP_CAJC were studied by field emission scanning electron microscopy (FE-SEM), and energy dispersive X-Ray spectroscopy (EDS). Electron transfer capacity at the interface of the PtNP_CAJC material was studied by cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) techniques. The PtNP_CAJC-GCE sensor was used for amperometric detection of nitrite. A lower limit of detection (LOD) and wide linear range for nitrite oxidation was found with the proposed sensor. We proposed a mechanism for sensitive detection of nitrite based on analysis of experimental findings of spectroscopic and electroanalytical techniques. We further utilized the proposed sensor for analyzing nitrite in tap water. The PtNP_CAJC-GCE electrode showed good reproducibility and stability.

Abstract ID: 234

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: room temperature superconductor, magnetic energy storage device

One-dimensional insulated polyacetylene superconductor candidate for Magnetic Energy Storage Devices

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Polyacetylene in its fully extended all trans configuration is expected to be a 1D metallic conductor if it has no bond alternation; a semi-conductor with a band gap if it has alternating bond lengths. It has not previously been possible to prepare polyacetylene in a fully extended conformation. Polyacetylene chains in proximity form chain to chain covalent bonds. The difficulties in preparation of polyacetylene is discussed in reference [3]

Urea inclusion compounds in which “guest” molecules are linear conjugated polyenes1,2,3 with terminal iodine atoms polymerize with broad band UV light. Raman spectra show new spectral features corresponding to longer oligomeric diiodo polyene chains. The frequencies and relative intensities of the two main Raman features parallel those observed for conjugated polyenes of known length. The progress of this polymerization can be monitored by the weight loss due to release of iodine which diffuses out of the inclusion compound.[3] When the weight approaches that for complete iodine loss based on the initial stoichiometry[1], it is observed that the Raman scattering disappears indicating the formation of very long polyacetylene chains for which the one-electron excitation cannot change molecular geometry appreciably. Synchrotron diffraction, polarized microscopy and inelastic neutron scattering indicate that the resulting polymer is present in channels in the crystalline material. It is anticipated3,4 that polymers that are sufficiently long that they exhibit two equivalent minima in their potential energy as a function of bond alternation will have a zero-point energy that is above the maxima in the potential by a large margin. This will result in a metallic conducting polymer in the absence of doping. Because the vibrations that modulate the conduction path are high, (>>kT) this structure is anticipated to be a superconductor. The fabrication of magnetic energy storage devices will be discussed.

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Abstract ID: 235
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Smart Composites
Keywords: Integrated smart windows, Electrochromism, Energy Storage

Highly efficient electrochromic electrodes based on composites of polyaniline with functionalized nickel oxide, zinc oxide and graphene quantum dots: Role of secondary interactions

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Smart window architecture based on low operating voltage is very efficient for energy saving, especially, when about 30-40% of primary energy in the world is being used for heating, cooling, ventilation, and lighting in buildings and vehicles.1 Smart windows by controlling the optical transmittance level, can control light and heat entering through the window and thereby reduces energy expenditure on air conditioning and lighting. Practically available devices are either based on viologens, which need continuous voltage supply to retain a color or on metal oxides which require high cost for synthesis and fabrication. Because of ample coloration, flexibility, ease of synthesis, cost effective fabrication, fast response and higher optical memory, the conducting polymers are now considered as appropriate materials for electrochromic applications.2 Among various studied conducting polymers, polyaniline is one of the most exploited material for electrochromic applications, but its lower electrochemical stability especially at higher potential, has always remained an issue for practical implementation. Here in the present work, we have tried to overcome this obstacle by introducing a secondary interaction between polyaniline chains and other stable materials like nickel oxide (PANI-fNiO), zinc oxide (PANI-fZnO) and graphene quantum dots (PANI-fGQD). With this approach, we are able to improve the stability of polyaniline upto 15,000 cycles along with parallel enhancement in optical contrast and coloration efficiency. Our composite PANI-fNiO exhibits transparent to black coloration with extended contrast throughout the visible spectrum as well as in near-IR and near-UV regions and superior coloration efficiency of 138 cm2 C-1. Composite PANI-fZnO shows very fast response of less than 1s with stability of 10,000 cycles. Composite PANI-fGQD, gives polychromic electrochromism with transparent to green to blue color with superior stability of 15,000 cycles. Such interaction manages to lower the nucleophilic attack on –N atom of pernigraniline, which is the main cause of polyaniline degradation at higher potential (> 0.6 V). Thus presented approach could be very beneficial towards improving the electrochemical stability of polyaniline. Moreover, we have further fabricated a prototype of all solid state electrochromic device based on PANI-fZnO as electrochromic layer and transparent gel electrolyte based on blend of polyvinyl alcohol and polyvinyl pyrrolidone.

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Abstract ID: 236

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Rare Earth-Based Hard Magnetic Materials

Keywords: Electrochemical synthesis, electroreduction, magnetic materials, rare-earth metals, ionic melts.

Electrochemical synthesis of magnetic materials based on rare-earth metals in ionic melts

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Intermetallic and refractory compounds of rare-earth metals with metals of the iron triad and boron have high magnetic characteristics. After the discovery of the unique magnetic properties of alloys such as SmCo5, SmPrCo5, Nd2Fe14B in the early 80s of the twentieth century, the demand for rare-earth metals and their compounds has increased sharply and continues to grow up to now [1]. The main way to obtain magnetically hard materials based on rare-earth metals is the melting of components at high temperatures, followed by dispersion in an inert atmosphere. These processes are complex and occur at high temperatures. In our opinion, one of the most promising methods of preparation may be electrochemical synthesis from molten halides.

The basis of the electrochemical synthesis of intermetallic (with metals of the triad of iron) and refractory compounds (borides, silicides) of rare-earth metals we have put together the processes of joint electroreduction of ions of rare-earth metals and metals of the triad of iron (iron, cobalt, nickel), as well as boron (silicon) in chloride melts alkali metals and their subsequent interaction at the cathode at the atomic level with the formation of micro-, submicro- and nanoscale powders of the phases of intermetallic and borides of rare-earth metals.

We have studied the processes of electrochemical reduction of lanthanum, gadolinium, neodymium, praseodymium, cerium, samarium, dysprosium, holmium ions in alkali metal chloride melts. The regularities of the processes of the joint electroreduction of the ignogous of rare-earth metals by fluoroborate, fluorosilicate ions and iron, nickel and cobalt ions in chloride melts at 973 K have been established. The electrochemical synthesis of micro-, sub-micro- and nanoscale iron powders, double borides of rare-earth metals with cobalt and iron has been implemented. The optimal parameters of the electrochemical synthesis of micro-, sub-micro- and nanoscale powders of borides, silicides, double borides, intermetallides of rare-earth metals and metals of the iron triad are determined: melt composition, electrolysis potential, cathodic current density, electrolysis duration.

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Abstract ID: 237
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Multiscale Modeling in Mechanics and Composite Materials
Keywords: Two-Phase Composites, Partial Sintering, Porosity, Elastic Properties (Shear, Bulk and Tensile Modulus, Poisson Ratio), Thermal Conductivity, Cross-Property Relation

Modeling the effective elastic constants and thermal conductivity of partially sintered isotropic two-phase composites

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The effective elastic constants (shear modulus, bulk modulus, tensile modulus and Poisson ratio) and the effective thermal conductivity of isotropic two-phase composites, for which the phase contrast is not too high, can be relatively well predicted using rigorous micromechanical bounds, i.e. the one-point (Paul-Wiener), two-point (Hashin-Shtrikman) and possibly three-point (Beran-McCoy) bounds. However, when these composites are porous, the possibilities of property prediction are much more limited. In particular, when the pore space surface is essentially concave, such as in partially sintered composites, there is no analytical prediction available that would provide sufficiently accurate a priori estimates of the porosity dependence of these properties. This study uses numerical modeling based on computer-generated 3D model random microstructures of two-phase composites (e.g. alumina-zirconia composites as typical examples) to calculate the effective properties and to check the validity of our cross-property relation between relative elastic moduli and relative thermal conductivity. Moreover, the direct (three-phase) numerical calculations are compared with the results of a two-step homogenization procedure in which first the effective properties of the dense two-phase composite are numerically calculated and then, in a second step, the porosity is taken into account (also by numerical calculation). The numerical results for the dense two-phase composites are compared with empirical mixture rules (including our sigmoidal averages) and analytical predictions (effective medium approximations), in particular the self-consistent approximation, which seems to reflect most closely the essential topological features of these microstructures. This work is part of the project “Partially and fully sintered ceramics - processing, microstructure, properties, modeling and sintering theory” (GA18-17899S), supported by the Czech Science Foundation (GAČR).

Abstract ID: 238

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Ceramic based composites

Keywords: Thermal / Electric Conductivity, Two-Phase Composites, Mixture Rules, General Power Mean, Fixed-Parameter Mean (Wyllie-Southwick model, Krischer model and Woodside-Messmer model), Volume-Weighted Sigmoidal Mean, Wiener Bounds, Hashin-Shtrikman Bounds, Ber

Empirical mixture rules and their application for estimating the effective conductivity and permittivity of isotropic two-phase composites

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The effective thermal conductivity, electric conductivity or permittivity of isotropic two-phase composites is bounded from above and below by rigorous micromechanical bounds, i.e. one-point (Wiener), two-point (Hashin-Shtrikman) and possibly three-point (Beran) bounds. As long as the phase contrast is small, these traditional contrast bounds provide rather satisfactory predictions, but for large phase contrast the prediction becomes increasingly worse. In this case, mixture rules can be a useful tool to estimate the effective properties, at least when the basic character of the microstructure is known (matrix-inclusion / coated-sphere, bicontinuous or symmetric-cell / granular) or at least to fit measured data for the purpose of meaningful interpolation. The first part of this contribution recalls the classical mixture rules based on the general power mean (which includes, apart from the volume-weighted arithmetic and harmonic means, also non-integer means, such as the Landau-Lifshitz mixture rule), for which a new formulation is given (which also includes the geometric mean or logarithmic mixture rule, i.e. the Lichtenecker relation). In the second part the fixed-parameter weighted means are summarized, which are known under the names Wyllie-Southwick model, Krischer model and Woodside-Messmer model. In the third part special types of floating-parameter means, viz. volume-weighted sigmoidal means, are discussed in some detail. It is shown that only the latter types of means are able to provide meaningful fits (or even rough predictions) for two-phase composites with granular microstructures. Finally it is shown that the volume-weighted sigmoidal means of both Wiener and Hashin-Shtrikman bounds tend to lie within the Miller bounds for symmetric-cell materials with spherical cells. This work is part of the project “Partially and fully sintered ceramics - processing, microstructure, properties, modeling and sintering theory” (GA18-17899S), supported by the Czech Science Foundation (GAČR).

Abstract ID: 239
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Ceramic based composites
Keywords: Alumina-Zirconia Ceramic Composites (ATZ), Partial Sintering, Porosity, Elastic Properties (Young's Modulus), Impulse Excitation (Resonant Frequency, Damping)

Investigation of partial sintering of alumina-containing tetragonal zirconia (ATZ) ceramic composites via temperature-dependent impulse excitation

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Alumina and zirconia ceramics are the most widely used oxide ceramics for many structural and functional applications, ranging from refractory bricks, furnace linings and thermal barrier coatings to transparent ceramics (impact-resistant windows), catalyst supports, filters, fuel cell membranes and biomaterials (bioinert implants). Composites of alumina and zirconia combine the high hardness of alumina with the high strength and fracture toughness as well as the lower elastic modulus (i.e. higher compliance) of zirconia. Moreover, adding alumina to tetragonal zirconia polycrystal (TZP) materials improves the resistance of the latter against hydrothermal aging, i.e. the low-temperature surface degradation due to the tetragonal-to-monoclinic phase transformation, while partial sintering is an easy way to retain porosity in the materials and thus to compensates the increase of elastic modulus (i.e. stiffness) induced by the addition of alumina. Based on extensive experience with impulse excitation measurements of elastic moduli and damping of alumina and zirconia ceramics, both at room temperature and at high temperature (up to 1200 °C), this study investigates the evolution of the elastic properties during partial sintering (during heating and cooling) and the temperature dependence of damping (during heating) of alumina-containing tetragonal zirconia (ATZ) composites (based on Tosoh TZ-3Y20A), prepared by uniaxial pressing and conventional sintering to different temperatures. In particular, the work investigates systematically the evolution of the Young's modulus when the original partial sintering temperature (1000–1400 °C) is exceeded. It is observed that in this case Young's modulus increases concomitantly with the continuing sintering. This work is part of the project "Partially and fully sintered ceramics - processing, microstructure, properties, modeling and sintering theory" (GA18-17899S), supported by the Czech Science Foundation (GAČR).

Abstract ID: 242

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Graphene, Mxenes and other two-dimensional materials for biomedical and healthcare applications

Keywords: Mannosylated chitosan nanoparticles, rHBsAg, Cytotoxicity

Novel approach to improve vaccine immunogenicity: mannosylated chitosan nanoparticles loaded with recombinant hepatitis B antigen as a targeted vaccine delivery system

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The recombinant hepatitis B virus surface antigen (rHBsAg) loaded mannosylated chitosan (MC) nanoparticles were studied as targeted vaccine delivery. The mannopyranosyl phenylisothiocyanate groups were coupled with chitosan (CS) and characterized by FTIR and 1H NMR. The MC nanoparticles were prepared by the ionic gelation method and characterized for physicochemical properties, cytotoxicity and antigenicity. The rHBsAg-loaded MC nanoparticles were shown spherical shape, mean particle size 246 ± 33 nm, zeta potential 25.6 ± 1.7 mV, loading capacity 12.2%, and encapsulation efficiency 90%. The In vitro release profile of rHBsAg-loaded MC nanoparticles exhibits an initial burst release of about 26% in the first 7days followed by a slow release of 25% in the subsequent 49 days and and release kinetic similar to the the Higuchi model. SDS-PAGE analysis confirmed the integrity of released rHBsAg and structural stability of the antigen during entrapment process. The rHBsAg-loaded MC nanoparticles were shown time and concentration dependent cytotoxicity in the MTT assay. In the present study, mannosylated low molecular weight CS was successfully prepared and an applicable procedure which can be implanted in industry with low production and initial funds introduced for the manufacture of biocompatible MC nanoparticles. It has been confirmed that the structural integrity of the encapsulated antigen was not damaged by encapsulation process. The MC nanoparticles prepared in this work were enable to protect entrapped rHBsAg and shown capability for use in vaccine delivery. Therefore, it seems that the rHBsAg-loaded MC nanoparticles are suitable candidate as new adjuvant and targeted vaccine delivery system candidate.

Abstract ID: 243
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Probabilistic modeling and reliability of composites
Keywords: ab-initio calculations, high-entropy alloys, HEAs, mechanical properties

Method for evaluating hardening in highly entropy equiatomic metal alloys

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A “hybrid” method is proposed - a combination of first-principle methods and a phenomenological approach for assessing the strength of a HEAs with a single-phase bcc and fcc structure.

It turns out that HEAs with a bcc structure are strengthened more strongly than alloys with a fcc structure, but under the condition that the number of elements is equal.

When adding a new element, the degree of hardening increases markedly.

The resulting analytical formula is of practical importance, because makes it possible to evaluate the degree of hardening for any single-phase equiatomic HEA, if the experimental data for the alloy are known — the type of crystal lattice and its parameter.

Abstract ID: 244

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Sensors and MEMS: Materials and Devices

Keywords: Supramolecular Polymer, Electron Transfer Kinetics, Nitrite Detection

Fabrication of Ni-Co based Heterometallo-Supramolecular Polymer Films and the Study of Electron Transfer Kinetics for the Nonenzymatic Electrochemical Detection of Nitrite

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Here, we report the synthesis of a bimetallic supramolecular polymer (SMP) for fabricating an electrochemical nitrite sensor, and study the reaction mechanism for the selective oxidation of nitrite by cyclic voltammetry (CV) simulation through evaluating the kinetic parameters. The symmetrical ligand bearing terpyridine moieties [4′,4′′′′-(1,4-Phenylene)bis(2,2′:6′,2′′-terpyridine)] were complexed with Ni (II), and Co (II) salts (Co:Ni:Ligand-0.5:0.5:1) (polyNiCo) for synthesizing the new heterometallo-SMP. The polyNiCo was characterized with the UV/Vis spectrophotometric titration, SEM, EDS, FT-IR, EIS, and CV techniques. The molecular weight of the polymer was determined from the intrinsic viscosity measurement, with the Mark-Houwink-Sakurada equation. While the spectroscopic data revealed the structural morphologies and properties of the polyNiCo; the electroanalytical characterization studies confirmed the high electrochemical activity and suitability of the polyNiCo heterometallo-SMP as an electrochemical sensor. The glassy carbon electrode (GCE) was used as the base for fabricating ployNiCo_GCE and used for detecting nitrite analyte through the oxidation process. The kinetics of the irreversible oxidation mechanism was studied using scan rate and pH variation methods. The electro-active surface area, electron transfer coefficient, heterogenous electron transfer rate constant etc. parameters were studied using the Butler-Volmer equations. We simulated CV of the nitrite oxidation process at the polyNiCo_GCE based on the analysis of these kinetic parameters of the electroanalytical experiments. The exceptional agreement between the experimental, and simulated CV confirmed the validity of the calculated kinetic parameters. Using CV and amperometry techniques we studied the effectiveness of the polyNiCo_GCE for detecting the nitrite analyte at different concentrations. The amperometry technique showed a wide linear range of 2.5 μM – 1.73 mM and limit of detection (LOD) of 0.45 μM. The sensor was also tested for interference, stability, and reproducibility. Real sample analysis was performed using both CV and amperometry techniques, and the obtained results were compared with the results from the standard solutions.

Abstract ID: 245

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Optical properties and spectroscopy of graphene and other two-dimensional materials

Keywords: Mixed alloy dichalcogenides, Raman, Shear mode

Raman scattering from Intralayer vs. Interlayer modes in alloy MoxW(1-x)S2

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Two-dimensional (2D) transition-metal dichalcogenide alloys have been recently attracting significant attention. Engineering their properties can be achieved by adjusting their metal and chalcogen atom contents to form ternary compounds.

The disorder induced alloying within the layer of mixed ternary-layered alloys leads to highly complex behavior of the intralayer modes [1]. Their composition dependent analysis of the Raman allowed modes require intricate consideration of the various possible arrangements within the layer. It is practically implausible to obtain with a commonly used MREI (modified random element isodisplacement) [1] the force constants of the various modes or to well-define the composition of the alloy, by analyzing its intralayer Raman spectrum.

The situation is different for interlayer modes Raman allowed shear mode, where disorder effects are not prominent due to the weak interaction between the layers in bulk MoxW(1-x)S2, ($0 \leq x \leq 1$) [2]. The absence of disorder effects in its interlayer motion (unlike for the intralayer motion) and the minor Mo/W shear mode composition dependence force constants enables the facile employment of the reduced monoatomic linear chain (MCM) model. Hence, with some alloy specific corrections, shear mode Raman scattering analysis may consequently be complementary to the electronic spectroscopy tools (XPS, EDS), commonly used for mixed alloy bulk composition characterization (Figure 1).

We will elucidate the nature of the two groups of modes by characterizing their compositional dependent response to low temperature and high pressure and will also demonstrate the effect of alloying on the modification of the resonant Raman behavior.

Abstract ID: 246

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: Tapioca, TiO2, Nanometric, Synthesis, Sol-gel

Influence of cassava starch (Tapioca) in the phases formation and optical properties of the TiO2 synthetized by sol-gel route

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Titanium dioxide (TiO2) is one of the of the most studied semiconductors because it has a wide range of promising energy and environmental applications, such as dye-sensitized solar cells, gas sensor, and photocatalytic water purification. Furthermore, it is well-known that the physicochemical properties of TiO2 are directly influenced by the synthesis method and, thus, over time several TiO2 synthesis methods have been presented by various research groups. Some of these methods value the search for materials obtained at a low cost, as well as linked to a sustainable perspective. Herein, we report on the synthesis of TiO2 nanostructures using a cassava starch (Tapioca) assisted by sol-gel route. Cassava starch is a low cost, renewable and abundant biopolymer which has been recently used as effective chelating agent in the synthesis of oxide nanoparticles. Thus, we synthesized a TiO2 samples using Tapioca, called of TiO2-T, and the other without using Tapioca, called only TiO2. The TGA results indicated that the optimal calcination temperature range to form TiO2 powders is 500-800ºC during 2 hours. All calcined samples were characterized by X-ray diffraction (XRD) and UV-Vis diffuse reflectance spectroscopy (DRUV). XRD indicate a nanometric character (13.8-163.6 nm) of both powders. However, it was observed that the use of Tapioca inhibited the formation of rutile at 600ºC when compared to the TiO2 prepared under the same conditions in absence of Tapioca. The anatase phase was recorded at all calcination temperatures in the TiO2-T, but with different percentages (6-100%). On the other hand, in the synthesis in absence Tapioca, the anatase phase was present up to 600ºC, corresponding to 87% of titanium oxide at that temperature. Moreover, at 600ºC the crystallite size of the anatase phase for TiO2 is twice that calculated for this same phase in the TiO2-T material. In addition, the DRUV spectra allowed the calculation of the forbidden band energy (Eg) in both direct and indirect transitions. These measurements demonstrated that for an indirect transition, Eg decreases, from 3.04 eV to 2.92 eV with the increasing of the calcination temperature for the TiO2 material. Similar behavior occurs for TiO2-T in the indirect transition, but the lowest Eg value occurs at 700ºC (2.86 eV). Regarding the direct transition, the band gap also decreases with increasing calcination temperature in both experiments, whose lowest values are reached at 700ºC which are 2.96 and 2.94 eV, respectively, for TiO2-T and TiO2. Changes in band gap values are probably associated with different percentages of anatase and rutile phases, as well as the crystallite size that each phase presents. Finally, this investigation highlights a simple procedure using a low cost, renewable and abundant material

(Tapioca) for the synthesis of titanium oxide. The results are promising pointed, considering the simplicity, low cost and sustainable perspective employed in this work.

Abstract ID: 247

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Nanoparticles, Nanowires, and 3D Structures

Keywords: topological insulator, spin-momentum locking, nanowire

Non-local spin transport in topological insulator nanowires

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The momentum and spin of charge carriers in the topological insulators are constrained to be perpendicular due to strong spin-orbit coupling. Sb2Te3 is one of the topological insulator materials with a bulk band gap of 0.28 eV and simple surface states consisting of a single Dirac cone in the band gap.1 We have synthesized single crystalline Sb2Te3 nanowires using low pressure catalytic chemical vapor deposition, via vapor-liquid-solid growth mechanism. Two levels of aligned e-beam lithography were used to pattern non-magnetic outer Au leads and two magnetic tunnel junction inner leads on individual Sb2Te3 nanowires. The tunnel junction leads consist of a free Py (Ni80Fe20) layer, whose magnetization determines the magnitude and direction of spin current injected into the Sb2Te3 nanowire.

Measurements of the device resistance between the two Au leads reveal that the Au/Sb2Te3 contact is ohmic. The two-point resistance measured between these contacts as a function of magnetic field shown exhibits positive magneto-resistance, originating from weak anti-localization of carriers in the Sb2Te3 nanowire induced by spin-orbit interaction. The weak anti-localization signal serves as evidence of a strong impact of spin orbit interaction on transport in the Sb2Te3 nanowire system.

We have also measured a non-local spin valve signal in Sb2Te3 nanowire channels. The symmetry of this non-local spin valve (NLSV) signal is dramatically different from that of a NLSV with a channel that lacks spin-momentum locking (such as graphene). Two parallel states of the injector and detector magnetic moments give rise to different non-local voltage values, which is never observed in conventional NLSVs. This unusual symmetry is a clear signature of the spin-momentum locking in the Sb2Te3 nanowire surface state.

Abstract ID: 248

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Optical properties of metals and non-metals

Keywords: Metal Insulator nanocomposites, Magnetic anisotropy, Exchange bias, SRSN, Electronic structure.

Electronic, Magnetic and Optical Properties of Shape Engineered Metal Nanoparticles and Si Nanostructures

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We present here electronic and magnetic properties of Ni and FeCo nanoparticles embedded in thin silica films and optical properties of Si rich silicon nitride films (SRSN). The salient results obtained can be summarized as (i) extraordinary hall effect with Hall coefficient (1000 times higher as compared to normal one) in Ni-SiO2 nanocomposites; (ii) tunable magnetic anisotropy in shape modified Ni-SiO2 nanocomposites; (iii) exchange bias effect to in FeCo-SiO2 nanocomposites due to spin flipping by thermal spike and (iv) tunability of photon emission from nanostructured SRSN films. Detailed electronic structure studies and first principle based calculations have been performed on nanocomposite films to understand the observed magnetic properties. A prototype magnetic field sensor based on nanocomposite is demonstrated.

The emission observed in the Si rich films is attributed to nanoscale a-Si:H inclusions. The enhancement is maximum for off-stoichiometric films and decreases as the compositions of a-Si and a-Si3N4 are approached, implying high density of non-radiative defects around. The diffusion of hydrogen in these films is also analyzed by Elastic Recoil Detection Analysis technique. Possible application of these films in photovoltaics have been outlined.

Key Words: Metal Insulator nanocomposites, Magnetic anisotropy, Exchange bias, SRSN, Electronic structure.

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Abstract ID: 249

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Nanocomposites

Keywords: Hybird Nano-structured Catalyst, Synergistic Catalysis, Photochemical route., nano-metal, selective hydrogenation ,

Synergistic Catalysis of nano-metal and semiconductor (metal oxides) molecular/atomic-layer film coated on the support of Novel Hybird Complex Nano-structured Pt Catalyst prepared by photochemical route

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Synergistic Catalysis of nano-metal and semiconductor (metal oxides) molecular/atomic-layer film coated on the support of Novel Hybird Complex Nano-structured Pt Catalyst prepared by photochemical route

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Herein, we report a novel strategy, which combine nano-metal with semiconductor (metal oxides) molecular/atom layer film coated on the support, to fabricate novel hybird complex nano-structured Pt/@-MeOx/SBA-15 catalyst prepared by photochemical route[1]. This hybird complex nano-structured Pt/@-MeOx/SBA-15 catalyst is a novel supra nano-structured catalysts, which nano-metal were anchored on the semiconductor (metal oxides) molecular-layer film coated on the support.

The novel hybird complex nano-structured Pt catalyst exhibited remarkable catalytic activity in the selective hydrogenation of benzaldehyde, conversion exceeding 99.9% was achieved with >99% selectivity. No decay in the activity was observed by 12 cycles. for the chemoselective hydrogenation of nitro compounds by 0.1wt% Pt/@-MeOx/SBA-15 catalyst, conversion achieved up to more than 99% with the selectivity of more than 99% .For the selective hydrogenation of p-chloronitrobenzene, it also obtained high selectivity(>99%) at complete conversion, the catalyst yields a TOF of 57588 h-1, about 2 orders of magnitude higher than that of the traditional Pt catalysts and 11.5-fold higher than the best result reported in the literature.

More importantly, the novel hybird complex nano-structured Pt catalyst exhibited the Synergistic Catalysis of nano-metal and semiconductor (metal oxides) molecular/atom-layer film coated on the support for the chemoselective hydrogenation of nitro compounds by Pt/@-MeOx/SBA-15 catalysts and for the selective hydrogenation.The superior performance can be attributed to the Synergistic Catalysis of nano-metal and semiconductor (metal oxides) molecular/atom-layer film coated on the support and the unique properties of hybird nano-structure.

Key Words: Hybird Nano-structured Catalyst, Synergistic Catalysis, Photochemical route., nano-metal , selective hydrogenation ,

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Abstract ID: 250

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Anodes and cathodes Materials

Keywords: Solid Oxide Fuel Cells, Specific Heat, Bulk Modulus, Manganites, Perovskite Cathode

Bulk Modulus and Thermal Properties of B-site doped La0.7Sr0.3MnO3−δ perovskite cathodes for intermediate temperature solid oxide fuel cells

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SrCoO3 − δ is an important parent compound of functional materials. Here we reported the thermal and elastic properties of La0.7Sr0.3MnO3−δ and SrCo1 − xMoxO3 − δ (SCM, x = 0.05–0.2) oxides as potential cathode materials for IT-SOFCs with LaGaO3 based electrolyte. The x = 0.05 composition of SrCo1 − xMoxO3 − δ is a promising candidate cathode for IT-SOFC application due to its good chemical compatibility, high conductivity and electrochemical performance [1]. It is also well known fact that the thermal compatibility of various component of a SOFC is equally important for the successful functioning of fuel cells in the operating range of the cell. In this paper we try to predict and tailor the elastic and thermal properties of some B-site doped perovskites in temperature range of 100k to 2000k. We investigate the various lattice distortions in these oxides AB1-xDxO3 and its effect on elastic and thermal properties of these perovskite manganites, especially Specific heat and thermal expansion of these complex oxides. The revealed data on Bulk modulus and Specific heat studied as a function of lattice distortions using a novel atomistic approach of Atom in Molecules (AIM) theory and Modified Rigid Ion Model (MRIM) are in closer agreement with the available experimental data for some concentrations of AB1 − xDxO3 . We propose the effect of distortions due to controlled doping at B-site as the tailoring tool to control and tune the thermal properties of these perovskite cathode materials.

Abstract ID: 251

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Materials for Memory and Computation

Keywords: RRAM, Switching characteristics, Endurance properties, HfO2

Switching Characteristics of Al-doped HfO2 Based Resistive Random Access Memory

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Existing non-volatile memory technologies like flash memories are charge storing memories and have now reached to its physical limits. To overcome the limitations of traditional memories and to bring advancement in new technologies like IoT and big data applications, the memories should be dense, power efficient and robust. Hence nano-scale memories which do not work on charge storing like FeRAM, MRAM, PCRAM, and RRAM have drawn a significant interest of researchers for future non-volatile memories. RRAM is a potential candidate for future memories due to its modest components, extraordinary compactness, low power, and exceptional scalability. The HfO2 based metal-oxide RRAM have been preferred by many researchers due to its high integration, fast operation speed, low power consumption, and high compatibility with advanced CMOS technologies.

In this paper, switching properties of Cu/Al:HfO2/Pt/Si RRAM devices were successfully demonstrated. After cleaning of silicon wafers, wet oxidation was done to grow SiO2 layer of 100 nm thickness on Si substrates to avoid the flow of the leakage current. Bottom contacts of Ti (50 nm) and Pt (20 nm), respectively, were deposited at room temperature using e-beam evaporation technique.The Al doped HfO2 thin film with a thickness of 10 nm was deposited using atomic layer deposition. Finally, different top electrodes of Cu (20 nm) were deposited using sputtering method. The crystallographic and surface morphological properties of metal oxide ZnO thin films were measured using XRD (PANalytical X'Pert Pro- 18-kW Cu X-ray diffractometer with CuKα radiation (λ=1.542 Å) and AFM (Multimode 8 SPM, Bruker) respectively. The Switching characteristics of all the devices were studied using B1500A Agilent semiconductor parameter analyzer. It has been observed that forming voltages and set voltages are reduced by using Al-doped HfO2 devices. It has been observed that the fabricated devices perform well without any degradation up to 3 x 103 cycles and both HRS and LRS do not show any degradation up to 104 s. The effects of Al doping on switching behaviour are explained on the basis of conduction filaments formed in HfO2 depending on dopants: oxygen vacancy (VO) filaments

Abstract ID: 252
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Nanocomposites
Keywords: Solvothermal method, Nanocomposites, Semiconductors, Heterogenous catalysis, Cotton fiber, Self-cleaning.

Plasmonic Hybrid Platinum-Titania Nanocomposites as Highly Active Photocatalysts: Self-Cleaning of Cotton Fiber under Solar light

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In the present work, a one-step, simple, efficient and low-cost strategy was demonstrated for preparing of highly stable hybrid platinum-titania (Pt@TiO2) photocatalyst by solvothermal wet chemical process 1. Platinum (Pt) in the metallic form combined with titania (TiO2) in the crystallographic anatase form has been manufactured using Dimethyl Sulfoxide (DMSO) as a solvent and surfactant using titanium(IV) butoxide and hydrogen hexachloroplatinate(IV) precursors. Full characterization of the hybrid nanomaterials including their morphology, crystalline structure and optical properties was determinate using different experimental techniques such as XRD, TEM and UV-Visible spectroscopy. TEM images showed spherically shaped Pt nanoparticles (NPs) of the diameter 5-10 nm with good particle size distribution. The EDXRF data revealed that Pt NPs are in metallic form. Optical investigation show that Pt@TiO2 NPs exhibits a good optical response under UV-visible light excitation compared to bare-TiO2. Furthermore, photocatalytic investigation of Pt@TiO2 colloids photocatalyst towards the photodegradation of diuron, as a model organic pesticide was reported. The hybrid Pt@TiO2 photocatalyst prove high-performance on the photodecomposition of the pesticide under solar light within only 60 min. In the other hand, the plasmonic hybrid Pt@TiO2 was incorporated into the cotton fabric to attain a modified fiber with high self-cleaning activity.

Abstract ID: 253

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Dielectric, Ferroelectric and Piezoelectric materials

Keywords: Polymer, Carbon nanotube, Hysteresis, Dielectric, Energy Storage

Hysteresis and dielectric properties of functionalized carbon nanotubes - polymer nanocomposite films

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In the recent time polymer nanocomposite films have attracted a great attention to the researchers due to their potential applications in electronic gadgets [1]. Due to semicrystalline nature of some polymers like polyvinylidene fluoride (PVDF) and polyvinyl alcohol (PVA), they are interesting for the applications in electronic device. On the other hand the carbon nanotubes (CNT) have versatile applications in nanoelectronics and they pogesses excellent mechanical and electrical properties along with high aspect ratio. The different functionalized (-COOH, -OH, -NH2) carbon nanotubes (f-CNT)-polymer films are prepared by using an economical and simple solution casting technique [2-3]. Samples are characterized by the X-ray diffraction, atomic force microscope image and two-dimensional fast Fourier transform spectrum analysis, which has confirmed the excellent alignment of f-CNT. The Raman spectra analysis has also confirmed the interaction between f-CNT and polymer and also suggested the formation of p-n junction between them. Hence the f-SWCNT embedded PVA films provide a high dielectric constant at lower f-SWCNT concentration due to their correct orientation. So these films may be used as high-k dielectric films. To illustrate the impedance spectroscopy of the nanocomposite films, we have proposed an impedance based battery equivalent circuit model. The current-voltage characteristic shows a good hysteresis behaviour of the fabricated capacitor of the composite films.

PVDF-f-MWCNT composite films have also shown the temperature dependent current-voltage hysteresis loop, which can be utilized as a non-volatile resistive memory device. To understand the conduction mechanism within the composite films, we have analyzed the measured current density data by using the existing different models. From the analysis, it is observed that during increasing mode of applied field the carrier conduction mechanism follows the Poole-Frenkel model and in the decreasing mode of applied field it follows the Schottky emission model. The trapping and detrapping of electrons takes a significant role in current conduction in this system. The ferroelectric hysteresis loop has been observed and the area under the loops represents the charge storage ability of the pure and composites films. Hence the energy storage density has been enhanced due to high aspect ratio and presence of functionalize group on the surface of MWCNTs and these materials can be utilized to developed polymer-nanocomposites in the field of energy storage application.

Key Words: Polymer, Carbon nanotube, Hysteresis, Dielectric, Energy Storage

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Abstract ID: 254

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Ceramic based composites

Keywords: Dielectrics, Ceramic, Multiferroics, BFO.

Structural, Electrical and Magnetic Properties of Bi(Fe0.7La0.3)O3 Ceramic

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La-modified BiFeO3 perovskite ceramic i.e. Bi(Fe0.7La0.3)O3 was synthesized by a well-established solid-state reaction technique. Examination of crystal structure, dielectric, ferroelectric and magnetic properties of polycrystalline Bi(Fe0.7La0.3)O3 ceramic was carried out. X-ray diffraction study uncovered rhombohedral-to-orthorhombic phase transition. Employing the X-ray peak broadening, the average crystallite size of the synthesized ceramic was calculated to be 30.43 nm. Detailed analysis of electrical and dielectric properties of Bi(Fe0.7La0.3)O3 was carried out in a broad frequency ranges from 1 kHz – 1 MHz and temperature 298K – 573K. The outcomes have displayed a collection of exciting result, concerning the structural and dielectric properties relationship. The low tangent loss values of the prepared ceramic are suitable for microwave applications. Complete findings of the outcome of grain and grain boundary in the resistive and capacitive characteristics of the material at nominated frequencies and temperatures by means of the impedance spectroscopy, have delivered numerous exciting and beneficial results for applications. Further, Vibrating Sample Magnetometer (VSM) was used to measure the magnetic field dependent magnetization in the ceramic.

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Abstract ID: 255

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Solar Cells

Keywords: Colloidal Quantum Dots, Macroscopic Profiling, Scanning Microscopy, Defect Characterization

Local Defects in Colloidal Quantum Dot Thin Films Measured via Spatially-Resolved Multi-Modal Optoelectronic Spectroscopy

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The morphology, chemical composition and electronic uniformity of thin-film solution-processed photovoltaics are believed to greatly affect device performance and stability, and, in recent years, spatially resolved characterization techniques based on scanning probe microscopy and frequency dependent carrierographies have been utilized to investigate such variations from micron to millimeter scale. However, such techniques are either limited in the field of view considering the active area of typical devices and the size of extrinsic defects introduced during fabrication, or in the ultimate resolutions imposed by the imaging system. Here, we demonstrate a micron-resolution 2D characterization method with millimeter-scale field of view which is capable of simultaneously collecting multi-dimensional photoluminescence spectra, photocurrent and photovoltage transients as well as full range J-V characteristics, which can then be used to extract more fundamental spatial-resolved device properties such as carrier mobilities, trap densities, quantum efficiencies, etc. With a high-resolution morphology mapping of the area of interest, we are able to examine the distribution and strength of the local variation of optoelectronic properties in colloidal quantum dot photovoltaic devices due to film defects, physical damage and contaminants across nearly the entire test device area, and the extent to which these variations can account for overall performance losses in the device. We find that macroscopic defects have effects that are confined to their localized areas, rarely prove fatal for device performance, and are not responsible for device shunting. Moreover, we show how quantitative analysis based on statistical partitioning methods of such data could automate and shed light on the fine variations of underlying physical properties such as mobilities and recombination strengths, and the mechanisms by which they govern device behavior.

Abstract ID: 256

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Experimental methods for Composite materials

Keywords: Resin impregnated paper, Bushing, curing cycle, winding paper, SEM

New experimental setup and procedure for construction of resin impregnated paper bushing

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New experimental setup and procedure for construction of resin impregnated paper bushing

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Infusion, impregnation, and curing process of an epoxy resin influences greatly the fabrication and, subsequently, the quality of resin impregnated paper (RIP) bushings as a composite electrical insulation. For appropriate manufacturing, accurate physical understanding and proper control of the process has a great importance in casting processes. Therefore, actual and efficient experimental approaches should be developed that can allow one to investigate the infusion, impregnation, and curing process directly during actual bushings construction. Accordingly, a new experimental pilot plant system for exploring a resin impregnated paper (RIP) bushing technology was designed, constructed and tested. This setup of equipment is similar to an industrial apparatus, but in an experimental scale. In this pilot study, all processes were performed corresponding to an industrial procedure. The sample technical specifications used for experiments were chosen based on a common commercial RIP bushing of the market. The main objective was to perform experiments, on the resin infusion, impregnation and curing processes in the paper condenser core of a RIP bushing. In this work, making various samples, different paper winding methods, molding procedures and curing cycles were evaluated using SEM micrographs and other tests. Finally, in addition of the construction of an actual bushing, important improvements were obtained in the case of filling and impregnation time reduction, curing time reduction, and bushing mechanical properties.

Abstract ID: 257
Symposium 4: Functional Composite Materials (FCM)
Poster/Oral Presentation
Topics: Multifunctional composites
Keywords: Hydrogel, Self-Vertical Migration System, Adsorbent

Development of shuttle adsorbent between the bottom and surface of water for adsorption of pollutants

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For various pollutants having a different specific gravity, the adsorbent having a similar specific gravity to the target pollutant is necessary to achieve enough contact time. Alginate hydrogel composite with controlled specific gravity and/or buoyancy was successfully developed, which can firstly sink in the bottom of water and then float up on the surface of water after the process of adsorption. The purpose of this work is to introduce a self-vertical migration system to the adsorbent for waste water treatment. The alginate hydrogel composite was prepared by using the alginate solution containing both glucose and yeast. The obtained beads firstly sank to the bottom of water, however, 30 min later, most of the beads floated up to the surface of water by generating carbon dioxide in the fermentation. This behavior repeated several times with the fermentation process acted as a float. In order to apply the unique property into the adsorbent, the removal of cesium ions in a water column was demonstrated by using Prussian blue modified alginate gel beads, which have a repeated vertical migration system. As the result, this adsorbent showed the faster removal of cesium than that by the adsorbent without the system. The system can be applied to the treatment of plenty amount of waste water which cannot be stirred and pumping. Therefore, the novel adsorbent developed in this study is expected to contribute to the environmental remediation.

Abstract ID: 258
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Polymeric composites
Keywords: Polymeric blend, Light-emitting layer, Charge-trapping, Förster resonance energy transfer

Host-guest polymeric blends for highly bright and efficient polymer light-emitting devices without the assistance of the charge-trapping effect

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Polymeric light-emitting materials have been developed recently as attractive solution-processable alternatives to conventional vacuum-deposited small molecules in organic/polymeric light-emitting devices, but they are still limited in terms of their performance, especially in terms of their low luminance, efficiency, and color instability. We report several noteworthy characteristics of a new blend of a host blue-emitting polyspirobifluorene-based copolymer and a guest yellow-emitting poly(p-phenylene vinylene) copolymer to compose a single light-emitting layer (EML). These host and guest polymers have nearly identical highest occupied molecular orbital levels of approximately 5.2 eV and lowest unoccupied molecular orbital levels of about 2.4 eV and 2.9 eV, respectively, minimizing the prevailing charge-trapping properties of their blends. Even in the absence of the charge-trapping effect, it is shown that very bright green electroluminescent (EL) emission with a maximum luminance level of ~142,000 cd/m2 can be realized for the blended host-guest EML at a moderate concentration (~5 wt%) of the guest polymer. The current efficiency was also observed and was found to be as high as approximately 14 cd/A, much higher than those (3.6~5.1 cd/A) of reference devices with pure host or pure guest polymeric EMLs. Moreover, there is a small change in the green color emission, with CIE coordinates of (0.35, 0.60) even at a high luminance level, showing good color stability of the EL emission from the blended EML. These significant improvements in the device performance are mainly attributed to the efficient Förster resonance energy transfer between the host and guest polymers in the blended EML. Together with its simple structure and easy processability, the high brightness and efficiency of our blended polymeric EML provides a new platform for the development of solution-processable light-emitting devices, advanced flat-panel displays, solid-state light sources, and/or electrically driven organic lasers.

Abstract ID: 259

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Photonic devices and applications

Keywords: Polyimide, Hole-transporting layer, Dark spots, Stability, Lifetime, OLED

Thin hole-transporting polyimide layers for very bright and efficient organic light-emitting devices with the reduced generation of dark spots

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Suppressing the device degradation caused by the formation of dark spots in organic light-emitting devices (OLEDs) is a promising route but remains challenging when attempting to develop long-lifetime OLEDs for various low-cost and high-performance flat-panel displays and light-emitting devices. The formation of dark spots is mostly attributed to ambient-induced electrical shorts, resulting in the diffusion of anode materials such as indium through the organic functional layer and local delamination of the metal cathode. In the present study, we develop a new thin layer (~20 nm) of functional polyimide (PI) and introduce it into OLEDs as a hole-transporting layer (HTL). This results in very bright and efficient electroluminescent (EL) performance, comparable to that of a control device. The device structure including PI HTL offers not only high device performance but also dense contact between the adjacent functional layers for effective hole-transport and sturdy structural stability during the operational phase of the device. Through systematic investigations of the PI HTLs, it is shown that the formation of dark spots in OLEDs can be significantly suppressed, which represents a critical step to realize long-lifetime OLEDs. This result confirms the anode-related origin of the dark spots; i.e., the indium-tin-oxide anode⁄organic interface plays an important role in the degradation. This study can offer promising directions for those involved in the effort to reduce the growth of dark spots while also providing useful insights into the development of low-cost, high-performance, and stable OLED displays and light-emitting devices.

Abstract ID: 260

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Graphene, Doped graphene, OLED, OLET, On/off ratio, Tunneling injection, Aperture ratio

FeCl3-doped graphene electrodes for the full-surface emission of vertical organic light-emitting transistors with high on/off contrast ratios and enhanced efficiencies

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The inherent structural complexity of active-matrix (AM) organic light-emitting diode (OLEDs) displays with their sophisticated procedures severely limits not only their size but also device performance, especially in significantly limited aperture ratios. Surface-emitting organic light-emitting transistors (OLETs) can provide an impressive solution for the next generation of AM displays by combining the capability of OLEDs to generate light with the electrical-switching functionality of a field-effect transistor into a single device structure. We report interesting characteristics of FeCl3-doped graphene as an active electrode for vertical-type organic light-emitting transistors (Gr-VOLETs). By introducing FeCl3 doping onto a graphene source electrode, the change in the work function of the graphene source induces variation of the potential barrier between the graphene source and an adjacent organic light-emitting semiconducting layer, allowing the switchable device performance of Gr-VOLETs to be improved significantly. We also reveal the role of the doped graphene in the Gr-VOLETs and the associated operating mechanism to explain the improved device performance via the effective gate-bias induced modulation of hole-tunneling injections at the doped graphene source electrode. Thus, the full-surface electroluminescent emission of the Gr-VOLET is effectively controlled by gate voltages with high luminance on/off ratios (~104), even at high luminance levels exceeding 500 cd/m2, together with current efficiencies much higher than those of control OLEDs. Our study highlights the FeCl3-doped graphene source electrode, offering significant improvements in the device performance of Gr-VOLETs.

Abstract ID: 261

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Sensor, Chemiresistive, reduced graphene oxide, Water, Lead

Sensing of Lead Using Graphene Based Chemiresistive Sensor

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Heavy metal contamination in water by mercury, lead, cadmium and arsenic has always been a serious threat to our environment as these elements are toxic and have a tendency to accumulate in our body and cause long term disorders. Accurate detection of these poisonous heavy metals is necessary and the most widely used techniques in this domain are inductively coupled plasma–mass spectroscopy (ICP-MS), and atomic absorption spectroscopy (AAS). However, these techniques are costly, require bulky instrumentation and real time detection is not possible. We have developed a simple and cost-effective chemiresistive sensor using reduced graphene oxide (rGO) as the sensing material for detection of lead (II) in aqueous medium. The sensor was prepared by first making a thin film of graphene oxide and the film was converted into reduced graphene oxide by thermal and chemical treatment. Selectivity towards lead was improved by using beta cyclodextrin. The sensor response, i.e. the change in resistivity in the presence of PbNO3 solution was recorded in the range of 1 to 600 ppm. This study shows considerable change in the resistivity of the sensing medium in the presence of salt solution. We were able to obtain around 60% change in resistivity for 50 ppm and around 15% change for 10 ppm for PbNO3 within 15 minutes. This sensor device offers practical solution for field detection of lead in case of industrial waste water and along with that further studies are to be undertaken for improving the detection limit of the sensor.

Abstract ID: 262

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Metal Oxide, ZnO thin film, Metal−Organic Frameworks (MOFs), ZIF-8, gas sensing, molecular sieve.

Fabrication of ZnO@ZIF-8 gas sensors for selective gas detection

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In this paper, zinc oxide nanorods encapsulated with a representative of the zeolithic imodazole based metal organic framework family (ZIF-8) is used as gas sensor material for the detection of hydrogen gas and benzene vapour. The material properties of this ZnO@ZIF-8 hybrid material was investigated by XRD, electron microscopy, Fourier transform infrared spectroscopy and gas sensing experiments. Selectivity and sensitivity of these thin films to various gases H2 and C6H6 were also studied. The ZnO@ZIF-8 sensor with the nanostructure showed a remarkable selective response to hydrogen gas as compared to the pristine ZnO nanorods sensor, while the ZnO sensor shows high sensitivity to H2 and C6H6. The ZnO@ZIF-8 sensor exhibits a significant selective response to hydrogen compared to the original ZnO nanorod sensor. This behavior can be attributed to the small pore aperture of ZIF-8, where H2 molecules it can easily spread through the ZIF-8 network and reach the ZnO surface.

Abstract ID: 263

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Electromagnetism

Keywords: Surface Dynamics, Electromagnetism, Differential Geometry

Does Invisibility Cloak Really Exist?

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Does Invisibility Cloak Really Exist?

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In this conference proceeding we will argue that long debated invisibility cloak theoretically is possible to exist. Recently we have proposed dynamic non-linear equations for moving manifolds in an electromagnetic field [1] and its consequent two dimensional surface dynamics equations [2]. The field is induced by a material body with a boundary of the surface. Correspondingly the potential energy, set by the field at the boundary can be written as an addition of four-potential times four-current to a contraction of the electromagnetic tensor. Proper application of the minimal action principle to the system Lagrangian yields dynamic non-linear equations for moving three dimensional manifolds in electromagnetic fields. The equations in different conditions simplify to Maxwell equations for massless three surfaces, to Euler equations for a dynamic fluid, to magneto-hydrodynamic equations and to the Poisson-Boltzmann equation and as we have already proven has few beautiful solutions [3, 4]. Using the equations of motions, here we can argue, that any system bounded by the moving surface, can be hidden from an electromagnetic field only if the surface dynamics satisfies specific, non-trivial solutions to the equations set (because of submission format does not allow, the equations are not provided in the abstract). To answer the question about existence of the invisibility cloak one needs to find the solutions to the equations, which is challenging problem. Though, we will indicate that few trivial solutions do exist, therefore the existence of the cloak is theoretically possible.

Key Words: Surface Dynamics, Electromagnetism, Differential Geometry

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Abstract ID: 264

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Mechanical and Thermal properties of graphene, Mxenes and other two-dimensional materials

Keywords: Mortar, Nanosilica, Compressive strength, Sulphate resistance.

Effect of incorporation of Nano silica on Properties of Mortar

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The importance of the cementitious materials in the construction industry is nowadays beyond any doubt; however, their variety of applications must not hide their complexity. Mainly properties such as mechanical , durability etc play an important role in the matrix formation of concrete, which is also effected by the presence or absence of superplasticizers. The basic aim of this study was to assess the suitability of using nano silica in pastes, mortars and concrete making it more advantageous and durable for the modern day construction. Exploration of nanotechnology in concrete on a commercial scale remains limited with few results successfully converted into marketable products. Nano silica is one such product. Nano silica modifies the molecular structure of mortar to improve the material's properties and particle placing in mortar can be improved by using nano silica which leads to densification of micro and nanostructure resulting in improved mechanical properties. Design and testing of mortar mixes (compressive strength, sulphate resistance and water absorption) with nano silica and optimization of the quantity of NS was carried out in present study. The conclusion was an approach to design mortar which will harvest the ideal way of applying nano silica in mortar, specified the available raw materials and the anticipated properties of the end-product. The above tests were carried out at various percentages of nS (0.5 to 1.5% @ 0.25%) used as partial replacement of cement and at various ages. Water absorption test at 28 days was performed for mortar specimens as per ASTM C642-13.Sulphate resistance tests at the ages of 56(28+28), 118(90+28), and 208(180+28) days was conducted for the mortar specimens as per ASTM C1012/1012M-13. It was observed that the consistency of mixes increased by approximately 9.5% in case of mortars without superplasticizer from control mix M-0 without nano-silica to mix M-5 containing 1.5% nano-silica whereas by approximately 14% in case of mortars with superplasticizer from control mix MS-0 without nano-silica to mix MS-5 containing 1.5% nano-silica. An increase in consistency and decrease in IST and FST was observed on varying the percentages of nano silica from 0% to 1.5% in both i.e. with and without superplasticizer in mortar. Flow table (mortar) decreased with increase in nano silica content. Presence of superplasticizer showed higher strength in mortar mixes. Optimum nS content was observed at 0.5% in without superplasticizer and 1% in superplasticizer mixes for mortar mixes with superplasticizer for compressive strength. Compressive strength increased with age in all mixes and higher strength was gained at early ages for mortar. Water absorption was minimum at optimum content of nano silica i.e. 0.5% and 1% in mortar mixes without and with superplasticizer, respectively. Positive effect was observed on addition of nano silica upto optimum content, when mortar specimens were tested for sulphate resistance.

Abstract ID: 265

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Fuel Cells

Keywords: Biological Reactor, Proton-Changing Membrane, Electric Energy

Microbian fuel cell electric power generation

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Microbial fuel cell (MFC) is a technology that consists of small biological reactors that have the function of converting the energy contained in the molecules of organic compounds into electrical energy or bioelectricity. One of the promising applications of these devices is the treatment of sewage combined with the recovery of energy contained in their molecules. In view of this, the present work aims at evaluating the generation of electric energy in a proton-changing membrane “H” (double chamber) type microbial fuel cell, which utilizes the sewage from the sewage treatment plant of the city of Volta Redonda / RJ as its organic source. Experiments have been carried out using the electrochemical impedance and polarization methods to evaluate the generated current and power values. Thus, it can be observed that the system was capable of treating the sewage effectively and produced energy (Maximum current densities = 0,693 mA.cm-2 and power = 0.693 mW.cm-2). Thus, this technology can work to harness the chemical energy of substrates while contributing to water pollution mitigation.

Abstract ID: 266

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Artificial photosynthesis

Keywords: CO2 reduction, Nano, photoconversion

CO2, Water, and Sunlight to Hydrocarbon Fuels: A Peak Joule-to-Joule Photoconversion Efficiency of 3.3%

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If we wish to sustain our terrestrial ecosphere as we know it, then reducing the concentration of atmospheric CO2 is of critical importance. An ideal pathway for achieving this would be the use of sunlight to recycle CO2, in combination with water, into hydrocarbon fuels compatible with our current energy infrastructure. However, the concept is intriguing such a technology has not been viable due to the vanishingly small CO2-to-fuel photoconversion efficiencies of known photocatalysts. Herein we report a photocatalyst, reduced blue-titania deposited with Cu-Pt bimetallic nanoparticles, that over 6 h generates a substantial amount of methane (3.0 mmolg-1) and ethane (0.15 mmolg-1) by CO2 photoreduction under equivalent solar spectrum (AM1.5) illumination. This activity (6 h) translates into a sustained Joule (sunlight) to Joule (fuel) photoconversion efficiency of 1% with a quantum efficiency of ϕ = 86%. The time-dependent photoconversion efficiency over 0.5 h intervals yields a maximum value of 3.3% (ϕ = 92%). Isotopic tracer experiments conducted using 13CO2 and H218O confirm the hydrocarbon products originate from CO2, and that water oxidation results in O2 generation. In addition, other advanced smart materials for CO2 works will be presented.

Abstract ID: 267

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Sensors and MEMS: Materials and Devices

Keywords: surface enhanced Raman scattering, machine learning, antibiotic susceptibility test

Metabolite Sensing as Signals of Cellular Processes

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Nanotechnology-based biosensors offer the ability to leverage a vast numbers of sensing elements per unit area. When coupled with a smart readout mechanism they offer the ability to mimic sensitive olfactory systems that relies on an interplay between sensitive receptors and synaptic processing of olfactory information. Surface enhanced Raman scattering (SERS) can simultaneously sense large numbers of small molecules, which can be differentiated based on their vibrational signature; thus it doesn't require capture agents such as antibodies and aptamers. Yet, SERS spectra are complex and difficult to attribute to individual molecules in a complex mixture. We first will present how 2-dimensional physically activated chemical (2PAC) assembly uses electrohydrodynamic flow to enable controlled molecular cross-linking between nanospheres. It overcomes long-standing challenges in reproducible nanomanufacturing of plasmonic 'nanoantennas' serving as ultrasensitive receptors. 2PAC achieves uniform (<10% RDS) billion-fold enhancements in elements spanning mm2. Large datasets can thus be acquired from 2PAC fabricated sensors that are critical for reliable training data for machine-learning (ML).

The SERS+ML approach enables early detection of biofilm formation. For example, supernatent from a culture from the opportunistic pathogen Pseudomonas aeruginosa are flowed over SERS sensors in a microfluidic channel. SERS+ML is able to detect biofilm formation as early as 3 hours after inoculation. Bacteria exposed to a bactericidal antibiotic were differentially less susceptible after 10 h of growth, indicating that these devices are useful for early intervention of bacterial infection. Further, we present that the complex vibrational signature of metabolites after antibiotic exposure provides the ability to distinguish between antibiotic resistant and susceptible strains. The complex metabolite vibrational signatures are used to distinguish antibiotic resistant from antibiotic susceptible P. aeruginosa. This is achieved after just 30 minutes of antibiotic exposure at the minimum inhibitory concentrations using linear discriminant analysis of SERS spectra from bacterial lysate.

Abstract ID: 268

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Stability of Nano, Micro and Macro Composite Structures

Keywords: Calcium hydroxide; Nanoparticles; Genomic instability; Inflammation and Mitochondrial damage

Genomic instability, inflammation and mitochondrial DNA damage induction by Calcium hydroxide normal and nano-nanoparticles

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Nowadays, there is increasing interest in using calcium hydroxide (Ca(OH)2) nanoparticles rather than normal sized Ca(OH)2 because of its higher antimicrobial activities. However, the genotoxicity of Ca(OH)2 nanoparticles has not been well investigated. Therefore, this study was performed to estimate the possible genomic instability, inflammation and mitochondrial DNA damage induction by normal and nano-sized Ca(OH)2 particles in mice. Oral administration of normal or nano-sized Ca(OH)2 particles induced DNA breakages and apoptosis causing genomic instability as a result of increased Calcium content, ROS , overexpression of inflammatory cytokines and MDA levels and decreased the GSH level and SOD and Gpx activities reversely proportional to Ca(OH)2 particles size. However, decreases in mitochondrial membrane potential concurrently with downregulated expression of POLG, POLG1 and TFAM genes were only observed in the brain and bone marrow tissues confirmed mitochondrial DNA damage. In contrast, the expressions of POLG, POLG1 and TFAM genes have been improved and mitochondrial membrane potential has not unchanged in liver tissues. Conclusion: single oral administration of normal or nano-sized Ca(OH)2 particles induced genomic instability and inflammation through ROS generation that exhausted the antioxidant defense system as well as impaired the mitochondrial DNA.

Abstract ID: 269

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: Mixed perovskite device, numerical simulation, device performance

Photovoltaic performances of eco-friendly mixed-cation inorganic perovskite solar cells

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Recently, solar cells based on organic-inorganic hybrid perovskite solar cells have received worldwide attention due to their outstanding properties as super high absorption coefficients, relatively high carrier mobility, and long carrier lifetime simple fabrication process [1]. The device efficiency of perovskite based on photovoltaic devices has been greatly increased from 3.8% in 2009 to over than 23.7%2. This value closely approximates with the efficiencies of traditional commercial devices as Si, GaAs, CdTe etc. In spite of the positive aspect, and great progress made on lead halide perovskite material, its instability and toxicity may handicap its potential use and its large-scale commercial production1. Thus, the serious environmental complications of lead require to search for some alternative candidate ecologic hybrid perovskite materials achieving the same high efficiency. To reduce the unhealthy effects caused by the toxic nature of Pb, researchers started to completely replace Pb with other less toxic divalent metals of the same group in the search of an alternative candidate for photovoltaic applications. In this perspective, Sun et al.3 reported that the doping Ge metal with Pb in 75% proportionally-mixed ratio can exhibit higher efficiency about 26%. We first performed drift-diffusion simulation to alter the Ge composition uniformly throughout the CH3NH3Pb1-xGexI3 absorber layer to ascertain the likely impact of varied band gap on device performance. Then a graded mixed perovskite absorber was analyzed, including back grading and double grading. The main objective of this work is to find an effective method to improve the perovskite device efficiency at the highest levels of device performance. This study can be expected to offer a promising route for more deeply understanding of operation mechanism and efficiency raise of perovskite solar cells.

Abstract ID: 270

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Advances in electrolyte and electrolyte additives

Keywords: Gel Electrolyte, Nmr, Polyurethane, Poly(Acrylonitrile), Conductivity

A Comparative Study on Performance of Polyurethane and PAN Based Gel Electrolytes

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Polyacrylonitrile (PAN) and partly cross linked polyurethane (PU) based gel electrolytes were investigated by impedance and 7Li nuclear magnetic resonance (NMR) spectroscopy. The ionic conductivity of the PU based gel electrolyte at room temperature is found to be in the order of 10-3 S/m, which is comparable to the PAN based gel electrolyte. NMR study shows that the environments of Li+ ion in both the gel electrolytes are identical. There are three kinds of Li environment: one in the solvent phase, the other in vicinity of polymer chain and the third in the nuclear magnetic dipole-dipole interactions with protons in the solvating molecules/polymer chains. The diffusion coefficient of Li ion in solvent phase of PU gel electrolyte is an order less than the PAN gel electrolyte. Even though the diffusion coefficient is less by an order, still the total conductivity of PU is comparable with PAN based gel electrolyte because of contribution of number of ions in solvent phase is much more than the ions in vicinity of the polymer chain. Moreover, the mechanical properties at high temperature and transparent nature makes the PU based gel electrolyte superior over PAN based gel electrolyte. In addition to the Li battery applications, PU based gel electrolytes can also be used in electrochromic device applications.

Abstract ID: 271

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: Structural analysis; Antiferromagnetism, Cyclic Voltammetry, Supercapacitors.

Complex magnetic structure, Magnetocapacitance and Asymmetric supercapacitor response in a non-oxide NiF2 system

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We discovered a colossal dielectric and supercapacitive response in NiF2, a non-oxide multifunctional system. It undergoes an anti-ferromagnetic transition near 68.5 K, superimposed with canted Ni spin driven weak ferromagnetic ordering, followed by a metastable ferromagnetic phase at or below 10 K. Near room temperature, NiF2 exhibits a colossal dielectric response reaching 104 with a low dielectric loss of <0.5 at frequencies >20 Hz. This is attributed to the intrinsic grain contribution in contrast to the grain boundary contribution in most of the known colossal dielectric materials. The activation energy for such temperature dependent relaxation is ~ 500 meV and is the main source for grain contribution. Further, NiF2 material is used as active electrode material in asymmetric supercapacitor device with activated carbon as negative electrode and the electrochemical properties were measured in 2-electrode device configuration. High capacitance of 175 F/g was realized for 1 A/g for the corresponding high potential window of 1.8V. Further, 93% of capacitance retention confirmed excellent cyclic stability of NiF2 based asymmetric supercapacitor device. We propose that our findings provide a new non-oxide multifunctional NiF2, useful for dielectric and supercapacitor research for its potential commercial applications.

Abstract ID: 272

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster/Oral Presentation

Topics: Graphene, Mxenes and other two-dimensional materials for biomedical and healthcare applications

Keywords: Chitosan; Nanoparticles; Echis carinatus venom; Adjuvant; Hyperimmune plasma.

A New Approach to Antivenom Preparation Using Chitosan Nanoparticles Containing Echis Carinatus Venom as A Novel Antigen Delivery System

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A New Approach to Antivenom Preparation Using Chitosan Nanoparticles Containing Echis Carinatus Venom as A Novel Antigen Delivery System

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In recent years, use of biodegradable polymers-based nanoparticles has received high interest in the development of vaccines delivery vehicles. The aim of study was to prepare chitosan nanoparticles (CS NPs) for loading Echis carinatus (EC) venom and evaluate their potential as an adjuvant and antigen delivery system on a pilot scale. CS NPs were prepared using ionic gelation method, and their characteristics were optimized. Venom-loaded CS NPs prepared under optimum conditions and traditional venom-loaded adjuvants were used to hyperimmunization of horse. Under optimum conditions, particle size, polydispersity index (PDI), and zeta potential of CS NPs were 127.9 ± 15 nm, 0.29, and +19.8 ± 1.92 mV, while those of venom-loaded CS NPs were 182.4 ± 20 nm, 0.35, +0.26.8 ± 1.98 mV, respectively. All CS NPs had integrated surface and good morphology. Optimum loading concentration of EC venom was 500 µg/mL. The loading capacity (LC) and loading efficiency (LE) were 87% and 94%, respectively, and release profile of venom-loaded CS NPs showed suitable correlation with Higuchi kinetics. Stability test showed good stability of the venom encapsulated in CS NPs. Furthermore, antivenom plasma obtained using the new antigen delivery system had significantly higher potency ($P < 0.05$) for neutralizing the venom than that obtained using conventional system. These results suggested that venom-loaded CS NPs could be a suitable alternative to conventional adjuvant for development antivenom.

Keywords: Chitosan; Nanoparticles; Echis carinatus venom; Adjuvant; Hyperimmune plasma.

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Abstract ID: 273

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Theory of graphene, Mxenes and other two-dimensional materials

Keywords: tunnel magnetoresistance, black phosphorene (BP), magnetic tunnel junction, first-principles, density functional theory, half-metallic ferromagnetic.

Study of effect of functionalization of black phosphorene on its spin-transport and magnetic properties

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First-principles spin-polarized density functional theory investigations are reported to understand the effect of functionalization (vanadium and titanium) on tunelling magnetoresistance (TMR) and spin-polarized transport of black phosphorene (BP) nanosheet based magnetic tunnel junction (MTJ) with 〖CrO〗_2 as electrodes. The results show, vanadium adsorbed black phosphorene based structure exhibits better spin filtration and high TMR, as compared to titanium adsorbed black phosphorene and pristine black phosphorene based structures. In addition, vanadium adsorbed black phosphorene nanosheet exhibits ferromagnetic behaviour with a magnetic moment of 2.6388 μ_b. The magnetic moment for pristine black phosphorene and titanium adsorbed black phosphorene nanosheets are reported to be 0.000007140 μ_b and 2.2 μ_b, respectively. Higher TMR, better spin filtration and ferromagnetic behaviour for vanadium adsorbed black phosphorene based structure opens up its possibility as spin filter (injector) in MTJs and other spin-based devices.

Abstract ID: 274

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Computational Electronic Materials

Keywords: magnetic tunnel junctions; spin density functional theory; spin-transfer torque; nonequilibrium Green's function; non-collinear device

Electronic transmission, tunnel magneto-resistance, and spin-transfer torque in magnetic tunnel junctions based on metal oxides: Fe/MnO/Fe, Fe/CaO/Fe, Fe/CoO/Fe, and Fe/BaO/Fe: comparative study with Fe/MgO/Fe

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In the past decades, flexible electronics research has helped in growing the market and the scientific growth due to their technological applications. The flexibility of these materials has revolutionized the conventional rigid electronics with the possibility to make them portable, bendable and lighter in weight. Furthermore, flexible electronics have improve from the latter advancement of organic and inorganic electronics in form of thin film and 2D technologies [1]. Sprintronics devices are among flexible electronics that have attracted attention due to their use in random access memory (MRAM), magnetic sensors and storage-hard-disk drives [2]. Nowadays, magnetic tunnel junctions (MTJs) are widely used in magnetic devices together with the giant magnetoresistance (GMR) materials. Due to the importance of the MTJs materials and their practical aspects, we propose to theoretically investigate a very attractive series of Fe/MnO/Fe, Fe/CaO/Fe, Fe/CoO/Fe, and Fe/BaO/Fe, using self-consistent NEGF- density functional theory (DFT) methods. We considered collinear and non-collinear spin-dependent transport properties, including electronic transmission, tunnel magnetoresistance, and spin-transfer torque. We compared the performances of the series to the widely studied crystalline MgO barrier [3] that reached a tunneling magnetoresistance (TMR) as large as 600% at room temperature.

Abstract ID: 275
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Nanocomposites
Keywords: Ion channels, plant cells, silicate, silicon nano particles

Silicon nanoparticles a new tool to increase plant growth and diminish stress

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It is well known that silicon, Si, is beneficial for plant growth and yield and also counteracts the negative effects of abiotic and biotic stresses. However, little is known about the mechanisms behind this. The plant-available Si in soils originates from amorphous SiO2 particles, phytoliths, similar to SiO2-nanoparticles (SiNP). Silicic acid, [Si (OH)4], has the ability to move across the root plasma membrane and is transported from root to shoot (Raven, 2001). In the present project we compared the uptake rate of potassium silicate with the uptake of silicon nano particles into cells of wheat by epi-fluorescence microscopy and the lysotracker Yellow dye HCK-123, which was incubated overnight. We found that SiNP, particles of silicon oxide, was taken up faster than potassium silicate into wheat root protoplasts, living cells without cell walls, and that the uptake rate depended on the particle size. In protoplasts from shoots the uptake rate was about the same rate when silicate or SiNP were added. Similar reults were found concerning Si uptake in ferrugreek at a whole plant level (Nazaralian et al. 2017). The present results suggest that the mesoporous nature of SiNP is like vehicles for silicon that easily can penetrate the cells and change the metabolic activities. Thus the SiNP could be an alternative, or even better, source of silicon fertilizer for crop plants.

Key words: Ion channels, plant cells, silicate, silicon nano particles.

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Abstract ID: 276

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Multifunctional composites

Keywords: Metal-Organic Framework, Photocatalysis, C-H Activation, Enzyme Mimic

Enzyme Mimicking Photocatalysis within Metal-Organic Architectures for Inert Csp3-H Bond Activation

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By incorporating the electron transfer pairs in both the ground and excited states into redox active Werner-typed metal-organic hosts with electronic acceptor/donor guest molecules, Prof. Duan's group has developed a promising protocol to mimic natural enzymatic systems in the redox transformations within a confined environment. The host-guest supramolecular systems fixed and isolated the donor-acceptor counter-pair with a short through-space separation, and without a through-bond electron transfer route. The confined electron transfer behavior was different from both the classical intermolecular or intramolecular photoinduced electron transfer processes that comply with Rehm-Weller or Marcus theory. It was proposed that this novel electron transfer behavior was helpful to stabilize the charge-separation pair, which enhanced the redox transformations in the ground and excited states. The intrinsic communication between the chromophore guest and the Werner host is the direct confined photoinduced electron transfer from the excited state of the chromophore to the host cage, which provided a bioinspired photocatalytic application of inert Csp3-H bonds activation within those metal-organic architectures.

Abstract ID: 277

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Silica, Photoluminescence, Phosphor, YAG, Light emitting diode

Inhibition of silica nanoparticles in solid-state-reacted Ce-doped yttrium aluminum garnet (YAG:Ce) phosphor ceramics by CO2 laser treatment

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Cerium-doped yttrium aluminum garnet (Y3Al5O12:Ce, YAG) is widely used in white light emitting diodes (WLEDs) as light converters to emit yellow light, namely photoluminescence. Especially the increasing use of high power blue LEDs to pump YAG:Ce will result in the degradation of chips as well as yellowing of resin or epoxy encapsulant materials due to poor thermal dissipation. Therefore, the developments of phosphor ceramics are recently proposed to replace organic-based WLEDs based on their excellent thermal conductivity and transparency properties. Silica (SiO2) like alumina to have a eutectic reaction with YAG at a lower temperature is usually added to form composite ceramics by a solid-state reaction (SSR) method. However, excess silica (5 wt%) was found to precipitate inside SSR YAG:Ce phosphor ceramics as seen in Figure 1, presenting a particle size range of 50 nm to 100 nm and a shape of dome on polygonal YAG:Ce grains. Owing to the fact of a smaller refractive index of silica (1.45) compared to YAG (1.83), it is expected to exhibit total internal reflection (TIR) at the interface of silica and YAG:Ce as converted yellowing light emitting from inside YAG:Ce. Here we propose one method of CO2 laser surface treatment for YAG:Ce ceramics to reduce silica precipitates by rapid heating and cooling, inhibiting the precipitation [1,2]. More details of precipitation mechanism and laser treatment will be discussed in the conference.

Abstract ID: 278

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Fiber reinforced Composites

Keywords: Graphene, Diels-Alder reaction, Self-healing behavior, CFRP composites

Self-healing agent grafted exfoliated graphene for introducing multiple healing capability in hybrid CFRP laminated composites

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2D nanostructure, high surface energy and aspect ratio, high surface area and superior mechanical properties of graphene make it an effective filler to tailor mechanical, thermal and electrical properties when reinforced in polymer composites. In this research, we have developed Diels-Alder (DA) based self-healing technique in CFRP composites by reinforcing surface functionalized graphene in the polymer matrix. Graphene was first oxidized through acid treatment to exfoliate and activate followed by functionalization with DA adducts, i.e. bismaleimide and furfurylamine. The successful functionalization of the graphene was confirmed from morphological, chemical, structural and thermal characterization. The DA adduct functionalized graphene showed ~57% improvement in tensile strength, ~79% in tensile modulus and ~11% in interlaminar shear strength when reinforced in CFRP composites. Most interestingly, we found ~87% in healing efficiency when tested with a double cantilever beam with several times healing capabilities. To date, it has been found that introduction of healing behavior in CFRP composites reduces the mechanical properties which are successfully overcome in this research. This study thus offers an emerging technology for self-healing of CFRP composites with functionalized graphene and can be a new threshold for future research in the development of self-healing polymeric composites.

Abstract ID: 279
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Nanocomposites
Keywords: Albizia procera derived carbon, nano-Mn3O4, nano-Co3O4, composite materials, electrochemical water oxidation

Preparation of metal oxide nanoparticle on Albizia procera leaves derived carbon for electrochemical oxygen evolution reaction

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Electrocatalytic splitting of water provides a potentially cost-effective, renewable, and clean path for the production of hydrogen gas. In this process, the efficiency of water oxidation (2H2O→4H++4e-+O2) is important. In the last few decades, the earth-abundant metal catalysts have been focused by the researchers that could possibly substitute the benchmark oxygen evolution reaction (OER) catalysts, i.e., Ru, Pt, and Ir. However, much attentions have been gained by catalysts based on earth-abundant metals (cobalt, nickel, and manganese) as several catalysts based on chalcogenides, phosphides, phosphates, and oxides of these elements have been developed for water splitting. Particularly, there have significant improvement in preparation of nanomaterials of oxides of these elements to meet the demands of electrochemical water oxidation. For proper utilization and saving the metal, simple preparation of nanomaterials including manganese oxide nanoparticles (MnOxNPs) and cobalt oxide nanoparticles (CoOxNPs) on cheap support materials is an interesting topic in OER research area. Here, we will present a simple and straight-forward thermal decomposition method to prepare Mn3O4NPs and Co3O4NPs on cheap and homemade Albizia procera derived carbon for electrochemical water oxidation. We employed direct thermal decomposition of Co(NO3)2·6H2O or Mn(CH3COO)2 at 300 □C without any pre-reaction to prepare nano-Co3O4, or Mn3O4 on the carbon. Various samples (electrocatalysts) were prepared by varying the amount of the Co or Mn precursor with the fixed amount of carbon using the same thermal decomposition parameters. After characterizing with X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), thermo-gravimetric analysis (TGA), X-ray photoelectron spectroscopy (XPS), and Raman spectroscopy, the prepared electrocatalysts were immobilized individually on the filter paper derived carbon electrode to study their electrocatalytic properties towards OER. Finally, we compared the obtained performances of the entire electrocatalysts and found optimum one for OER. Due to straight-forward and simple preparation, low cost, efficient electrocatalytic property, and good stability, the optimum nano-Co3O4 or nano-Mn3O4-coated carbon composite could be counted as promising materials for electrochemical water oxidation.

Abstract ID: 280
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Nanocomposites
Keywords: Nanotheranostics, Gold Nanodandelion, Anti-obesity, Orlistat, Mesoporous Silica Nanoparticle

Minimalism Is the Practical Fashion of Nanotheranostics

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From industrilization's eye view on nanomedicine, the simplicity seems to be the key to successful translation. Herein, we present some of our past and current works as examples of why Minimalism Is the Practical Fashion of Nanotheranostics:

(A) In Cancer Phototherapy, nanoparticles have played a key role in the enhancement of the radiation therapy by acting both as a therapeutic as well as a carrier for other therapeutics. The use of nanomaterials as radiosensitizers has made significant progress in recent years. In our work, with specific tuning of annealing process during our LaF3:Tb@SiO2 and Y2O3:Eu@SiO2 syntheses, we could produce the first so-called "photosensitizer-free" x-ray nanoscintillators" that are capable of generating significant quantities of cytotoxic reactive oxygen species (ROS) under low-dose, low-energy x-ray exposure, and possessed of several important advantages over the conventional XPDT. Another example is a new type of biodegradable flower-like gold nanodandelion (GND). It displays important features and some are the first of its kind: (1) large scale green synthesis of GND with high monodispersity; (2) cellular/physiological degradability of GND leading to its disassembly into debris, which is favorable for efficient body clearance; (3) precision control of the chemicophysical properties of GND including shape, petal number and size, all can be judiciously fine-tuned by the synthetic parameters; (4) highly efficient radiotheranostics of GND encompassing better enhanced CT contrast and pronounced x-ray induced ROS generation than conventional spherical AuNP; (5) Switchable utility for XPDT and near-infrared I/II photothermal therapy (PTT).

(B) In Anti-Obesity Nanotechnology, Obesity can cause many chronic diseases, such as cardiovascular disease, diabetes, and other life-threatening ailments. In the anti-obesity market, Orlistat is the main active ingredient of many existing weight-controlling drugs to reduce fat absorption, such as Xenical, It acts as a lipase inhibitor to reduce the degradation and absorption of gastrointestinal fats, resulting in excess fat being excreted as steatorrhea, one of the unpleasant side effects. In this study, we simply and straightforwardly exploited the high surface area (800-1000 m2/g) of mesoporous silica nanoparticle (MSN) to adsorb oil and create oil gelatinization/solidification, thus to minimize/eliminate steatorrhea. MSN is a good candidate for large-scale production, and no surface modification is needed to exert its function in this regard.

Abstract ID: 281
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Nanocomposites
Keywords: Co3O4 nanowires, polypyrrole, composite materials, electrochemical water oxidation

Preparation and characterization of nano-Co3O4 and polypyrrole composite materials for enhanced electrochemical water oxidation

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Water oxidation is one of the most important research area for storing and using green energy in these days. Nano-Co3O4 were used for electrocatalytic water oxidation due to its promising features for better performance and lower cost. However, the enhanced electrochemical water oxidation performances of the semiconductors, nano-Co3O4 is expected by mixing them with other types of high conductive materials. Conductive polymers would be one candidates to achieve this goal. Here we present our recent developed novel nano-Co3O4 and polypyrrole composite materials for enhanced electrochemical water oxidation. We chose polypyrrole as support of nano-Co3O4 to obtain high active site of nano-Co3O4 with high conductivity. To prepare the composite materials, initially Co3O4 nanowires were prepared by simple thermal decomposition of Co(NO3)2·6H2O as per our earlier report [1]. Then they were mixed with chemically prepared polypyrrole in different ratios to obtain the optimum electrocatalyst for water oxidation. Morphological and chemical characterization of the prepared materials were performed using scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), X-ray photoelectron spectroscopy (XPS). After immobilizing them individually on fluorine doped tin oxide substrate, their electrocatalytic properties toward water oxidation were performed. By comparing the obtained electrocatalytic properties, the optimum ratio of Co3O4 nanowires and polypyrrole for efficient water oxidation was determined. Due to good stability, efficient electrocatalytic property and low cost, the optimum nano-Co3O4 and polypyrrole composite could be represented as a promising material for water oxidation.

Abstract ID: 282

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Solar Cells

Keywords: Vanadium Oxide, Atomic Layer Depositionm, Si Heterojunction Solar Cell

Charaterization of Atomic-Layer Deposited Vanadium Oxide for Si Heterojunction Solar Cells

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Silicon heterojunction (SHJ) solar cells can achieve high efficiency with simple structure. Vanadium oxide (VOx) is known as one of the hole-selective layer materials. To achieve higher efficiency, we need to make fine hole-selective layer. Atomic layer deposition (ALD) allows us to deposit thin film uniformly. We report on VOx deposition on Si substrate by ALD using vanadium tri-isopropoxide (VTOP) as precursor and H2O as reactant. Film growth behaviors were measured by ellipsometer to find the saturation growth condition for deposition of VOx by ALD. The growth rate of ALD VOx was 0.3 Å/cycle between 100 and 150 ℃. Oxidation states of vanadium in deposited and post annealed VOx films were analyzed by x-ray photoelectron spectroscopy (XPS). After deposition of VOx on Si wafer, we measured its carrier lifetime and Voc by quasi-steady-state photo conductance (QSSPC). We confirmed that its passivation characteristics are improved with lifetime of 55.26 μs and Voc of 654 mV at 90 ℃. It shows that ALD VOx thin film can be applied to SHJ solar cells.

Abstract ID: 283

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Photonic devices and applications

Keywords: Metal-Organic Framework, Single-Molecule Diode, Nanoreactor, Photocatalysis, Late-Stage Functionalization

Single-Molecule Diode within Metal-Organic Composite Nanoreactor for Photo-Metal Dual Catalytic Late-Stage Functionalization of Drugs

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As inorganic-organic hybrid materials, metal–organic frameworks (MOFs) exhibit the combined advantages of transition metal-type catalysts and organic molecular photocatalysts. The excited states, charge separations, and charge mobilities of MOFs remarkably influence the results of MOF-based photocatalytic systems, which reflect varying degrees of characteristics of inorganic semiconductor-like nodes and organic ligands and require highly oriented electron flows between transition-metal sites and photoresponsive centers. Herein, we report a novel tuning strategy by constructing single-molecule diode array within metal-organic frameworks for rectifying the excited-state and ground-state electron transfer routes in the productive manners, circumventing the usual fluorescence quenching of chromophores by transition-metal ions in the homogenous phases. Steric repulsion induced twisted conjugative chromophore–high valent transition metal junction together with the high polarity of the carboxylate–transition metal node within the framework ensure the unidirectional charge mobility for furnishing the photoredox–transition metal dual-catalytic cycles. This new noble-metal-free, recyclable metal-organic composite nanoreactor enables its value-added application in the late-stage functionalization of pharmaceuticals under photoirradiation.

Abstract ID: 284
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Bio-composites
Keywords: Boundary Element Method, Bio-composites, Thermomechanical Interactions, Nonlinear Dual Phase Lag Bio-heat Transfer, Functionally Graded Anisotropic Soft Tissues

Boundary Element Thermomechanical Modeling of Fractional-Order Nonlinear Dual Phase Lag Bio-heat Transfer Problems in Functionally Graded Anisotropic Soft Tissues

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The main objective of this paper is to contribute for increasing development of bio-composites applications according to our boundary element modeling for describing thermomechanical interactions in functionally graded anisotropic (FGA) soft tissues. The governing equations of current model are briefly presented, including the time fractional-order nonlinear dual-phase lag bioheat transfer model and Biot's model. These highly complex governing equations are solved using the boundary element method (BEM), which is an efficient and accurate method for modeling of bioheat distribution in FGA soft tissues, because it only requires discretizing the boundary of the problem, and then dealing with FGA soft tissues problems involving complex shapes. Also, it needs low CPU usage and low RAM usage. The general boundary element method (BEM) based on local radial basis function collocation method (LRBFCM) has been used for solving the time fractional-order nonlinear dual-phase lag bioheat transfer model. Then, the displacement and stress distributions can be achieved by solving the mechanical equation using the convolution quadrature BEM. Numerical results demonstrate the validity, efficiency and accuracy of our proposed modeling technique.

Abstract ID: 285

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: supercapacitor, hybrid, LDH, rGO, nanocomposite

Nanocomposite of Ni.Co LDH/rGO based electrode for high performance supercapacitor application

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Recently, increasing population and economic development led to higher consumption of fossil fuels and due to limited sources of fossil fuel, society needs clean and renewable energy sources along with advanced technology to store such energy in device. In that context, supercapacitor attracted major attention of research world due to its characteristics such as high power density, environment-friendly, excellent stability and wide operating temperature range. In this paper, we developed Ni.Co LDH/rGO nanocomposite deposited on stainless steel foil electrode for supercapacitor by using simple one-step hydrothermal method. Direct deposition of Ni.Co LDH/rGO on steel foil gives binder-free electrode for high-performance supercapacitor. Prepared nanocomposite characterized to study crystallographic and morphological study under XRD, FESEM and TEM. The XRD peaks exhibited showed that the formation of uniform composite of Ni.Co LDH/rGO. SEM results reveal that Ni.Co LDH nanosheets vertically grown on rGO sheet. Surface area and particle size were measured by using BET techniques and it is 5-8 nm. The cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD) techniques are used to evaluate electrochemical performance. The nanocomposite of Ni.Co LDH/rGO deliver superior electrochemical performance and exhibited specific capacitance of 2987 Fg-1 at current density of1 Ag-1 with capacitance retention of 85% after 2000 cycles. Asymmetric supercapacitor fabricated using prepared electrode Ni.Co LDH/rGO deposited on steel foil as a positive electrode and Fe2O3 deposited on steel foil act as a negative electrode. The specific capacitance of 156 Fg-1 was obtained for fabricated asymmetric supercapacitor along with 45 Wh Kg-1 at a power density of 1500 W Kg-1. The obtained characterization results suggest that prepared material is a potential candidate in the practical application of supercapacitor.

Abstract ID: 286

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Solar Cells

Keywords: Laser doping, Selective emitter, Borosilicate glass

Laser doping of borosilicate glass for selective emitter formation

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Selective emitter formation technology is an effective way to improve the performance of silicon solar cells. The selective emitter can reduce the contact resistance of the electrode and the silicon by selective doping only the portion forming the electrode in a low concentration emitter to a high concentration. In this study, a laser doping method was used to form a selective emitter. Laser doping processing has many advantages, such as a simple and low temperature process, and high throughput. A borosilicate glass (BSG) layer having a sheet resistance of 100 Ω/sq was grown on the furnace and then doped with a UV laser having a wavelength of 355 nm. After laser doping only a small part of the boron is diffused from the BSG layer into the silicon. The selection area has a sheet resistance of 35-50 Ω/sq. As a result of laser doping, the depth of diffusion increases with increasing power and the sheet resistance decreases with increasing current.

Abstract ID: 287

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Computational Electronic Materials

Keywords: Heusler compounds, DFT, ScPtBi, Spin-Orbital Coupling, Topological Phase

Effect of Spin-Orbital coupling on Electronic and Vibrational properties of ScPtBi: A First Principle Study

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Heusler compounds are one of the versatile class of compounds due to their large number of technological applications [1]. In this article, the electronic and vibrational properties of half-Heusler compound ScPtBi have been studied by using first principle calculations including the spin-orbit coupling (SOC). The plane wave pseudo-potential method within density funtional theory (DFT) is used to compute these properties. The SOC has a considerable effect on electronic band structure of ScPtBi leading to band inversion without breaking any symmetry. This band inversion results in emergence of topological phase in ScPtBi. The density functional perturbation theory (DFPT) is imployed to plot the phonon dispersion curve and phonon density of state and zone center frequencies with and without SOC are also compared.

Abstract ID: 288

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Theory of graphene, Mxenes and other two-dimensional materials

Keywords: Electronic transport in AB-bilayer Graphene, Kubo formalism of conductivity, twisted multilayer Graphene nanostructures

Electronic transport in AB-bilayer and twisted bilayer graphene nanostructures

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Abstract: Recently graphene AB-bilayer, twisted AB-bilayer and also graphene trilayer nano-structures exhibited peculiar combination of linear (near Dirac Point) and parabolic electronic band structure, tunable band gap and localization of the Dirac quasiparticles and also emergence of superconducting state. The twisted version of AB tacked bilayer and trilayer graphene nano-structures indicated a marked difference in the electronic properties among other existing two dimensional electronic materials. The numerous experimental data on multilayer graphene nanostructures related to electronic structure and transport behavior are now available and one need to develop microscopic theoretical understanding to interpret the experimental observations. We have attempted theoretical modeling of electronic structure and transport behavior in bilayer and trilayer Graphene nanostructure and also their twisted version. The Green's function many body techniques within plausible approximations guided by recent theoretical and experimental studies have been employed based on model Hamiltonian containing various intra and interlayer contributions and correlation effects. We have analyzed in detailed the electronic density of states, quasiparticle energies, as well as electrical conductivity of these systems within Kubo formalism by calculating current–current correlation function in linear response for AB staked bilayer Graphene keeping influence of onsite Coulomb interaction to the first order guided by existing experimental and theoretical works. The recent development related to experimental and theoretical issues of unconventional Superconductivity in AB-bilayer and twisted trilayer graphene will also be highlight.

Key words: Electronic transport in AB-bilayer Graphene, Kubo formalism of conductivity, twisted multilayer Graphene nanostructures

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Abstract ID: 289

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Smart Composites

Keywords: biofilm, chitosan, electrophoretic deposition, gallium, postarthroplasty infection, pulsed electromagnetic field, Staphylococcus aureus, Staphylococcus epidermidis.

Bactericidal activity of Gallium-doped chitosan coatings against staphylococcal infection

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INTRODUCTION: This study was to develop a new class of Gallium (Ga)-doped Chitosan (CS) coatings fabricated by electrophoretic deposition (EPD) that promise new opportunities in staphylococcal infection therapy.

METHODS: Titanium sheets (Ti, grade 2) were used as cathode in an electrophoretic deposition cell: electrodes were positioned at distance of 10 mm [1] in a lab made EPD cell.

Biofilm formation on EPD CS/Ga coatings by Staphylococcus epidermidis and Staphylococcus aureus, which are the main strains involved in post-arthroplasty infections was assessed. The codeposition of antibacterial agent was effective. Lastly, the influence of Pulsed Electromagnetic Field (PEMF) on the bactericidal activity of CS/Ga coatings was investigated in vitro. To this end, the coatings were incubated with S. epidermidis and S. aureus and exposed to the PEMF using two different frequencies and times.

RESULTS: Ga loaded into CS matrix reduces biofilm viability by up to 86% and 80% for S. epidermidis and S. aureus strains respectively. Biofilm viability for S. epidermidis was decreased up to an additional 35 to 40% in the presence of low and high frequency PEMF, respectively. Biofilm viability by S. aureus was not further reduced in the presence of low frequency PEMF but decreased up to an additional 38% at high frequency PEMF.

DISCUSSION & CONCLUSIONS: This study has established that a combination of pulsed electromagnetic fields with the antibacterial agent, improves bactericidal activity of Ga against S. epidermidis strain 14990 and S. aureus strain 12600. The new integrated approach could reduce the incidence of infection in orthopaedic implant applications..

Abstract ID: 290

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Polymeric composites

Keywords: Poly (brilliant cresyl blue), Reduced Graphene Oxide; Nitrite Sensor

Poly (brilliant cresyl blue)-reduced graphene oxide modified activated glassy carbon electrode for the fabrication of nitrite sensor

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In this article we studied a modified electrode, used as an electrochemical sensor (ECS) with the help of simple electrochemical experiments, and affirmed the underlying chemistry by means of the theoretical and computational (CP) analysis. The ECS was developed by the electrodeposition of poly (brilliant cresyl blue) (PBCP) on an electrochemically reduced graphene oxide (ERGO) at the activated glassy carbon electrode (AGCE) (AGCE/ERGO/PBCB). The AGCE/ERGO/PBCB sensor was characterized through electrochemical and electron microscopy methods; while the CP methods were used for understanding the molecular interaction processes. The analysis of the characterization data supported our assumption, that the AGCE is the better platform for the optimal electrochemical reduction of GO, compared to the GCE for the purpose of the electropolymerization process. The AGCE/ERGO/PBCB was then used for the sensitive nonenzymatic detection of the nitrite species in the acidic medium using amperometric and cyclic voltammetry (CV) techniques. Analysis of these experimental, and CP data revealed that the AGCE, ERGO, and PBCB interacted with each other through the parallel-displaced and sandwich types π – π stacking, and electrostatic interactions. H•••O−H, and H•••N−H hydrogen bonds between the functional groups of AGCE and ERGO also promoted the electron transfer process. The microscopic data suggested the possibility of both horizontal and vertical growth of the folded nanosheet like PBCB, which was further confirmed from the electrostatic interaction data. Through pH variation experiment, and CP analysis, we confirmed that PBCB acted as the mediator for the nonenzymatic oxidation of the nitrite species at the AGCE/ERGO/PBCB system. The kinetic parameters study of the polymer and nitrite oxidation process revealed the surface coverage was 2.09 x 10-9 mol/cm2, electron transfer rate constant as 0.006 cm/s, and effective surface area of 0.144 cm2 for the AGCE/ERGO/PBCB. The limit of detection (LOD) was 60 ± 0.54 nM, with sensitivity of 0.36 μA/μM. The ECS was also tested for interference, stability, reproducibility, and real sample analysis.

Abstract ID: 291
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Nanocomposites
Keywords: Thermoregulation, nanocomposites, nanocoatings, flame retardancy

Application of functional TiO2/Hollow Glass Microsphere nanocomposites on cotton for heat absorption and flame retardancy

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It has been reported that around 30% of total heat loss and gain of commercial and residential buildings indoor space takes place through windows. This leads to imposing extra energy consumption loads for adjusting the temperature of indoor space in different seasons of the year. It is estimated that this accounts for 20-40% of total consumed energy bills [1]. To tackle this issue, this research developed functional nanocoatings containing TiO2 nanoparticles and Hollow Glass microspheres (HGMs) to the surface of curtain fabrics and the impact of this treatment on heat regulation performance and flame retardancy of curtains was assessed. The obtained results showed that the presence of an optimized amount of HGMs on curtains significantly reduced the thermal exchange rate between the building's indoor space and outside environment. Moreover, the developed composite coatings on curtain fabrics resulted in flame retardancy and excellent UV protection both of which are necessary for having functional curtains. These findings can dramatically contribute to lowering the energy consumption in buildings and improving the well-being of users.

Abstract ID: 292

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Solar Cells

Keywords: atomic layer deposition, carrier selective contact, heterojunction, MoOx, silicon solar cell

A Study on MoOx Thin Film Using ALD for Efficiency Improvement of Heterojunction Si Solar Cell

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The MoOx thin films deposited using ALD as a hole-selective, dopant-free contact to n-type silicon MoOx as a high work function metal with a low density of states at the Fermi level originating from a defect band inside the band gap. The MoOx thin film is mainly used as a barrier film or a passivation film by selectively extracting holes in silicon. MoOx was deposited from 5 nm to 15 nm in carrier selective contact structure using ALD (Atomic Layer Deposition). quasi-steady-state photo-conductance (QSSPC) technique can be very useful to assess the intrinsic VOC potential of undamaged device structures. The obtained open-circuit voltages (VOC) increased at 750mV. X-ray photoelectron spectroscopy (XPS), depth profiling through Auger Electron Spectroscope, and HR-TEM measurements showed chemical bonds and properties shows that the Mo+6 state is dominant in the MoOx thin film. Instead of using a p-type amorphous silicon layer, high work function MoOx films as hole selective contact are applied for heterojunction silicon solar cells and the best efficiency yet recorded (21 %) with iVOC 726 mV, VOC 730 mV, JSC 38.5 mA / cm2, FF 75.1% in HIT cell structure of ALD-MoOx thin film. . By obtaining the solar cell efficiency of 21%, MoOx thin films were deposited using atomic layer deposition, which showed the possibility of improving the efficiency of heterojunction solar cells by improving hole selective contact and passivation.

Abstract ID: 293

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Production and characterization of composite materials

Keywords: Cellulose acetate, Cation exchanger, Nanocomposite, Sol-gel method

Synthesis and Characterization of Cellulose acetate titanium (IV) tungstomolybdate Nanocomposite Cation Exchanger for the Removal of Selected Heavy Metals from Aqueous Solution

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ABSTRACT

Cellulose acetate titanium (IV) tungstomolybdate nanocomposite cation exchanger was synthesized by sol-gel method by incorporating cellulose acetate polymer into inorganic exchanger, titanium (IV) tungstomolybdate. Different techniques including FTIR, XRD, TGA SEM and BET were used to characterize the exchanger. The Cellulose acetate titanium (IV) tungstomolybdate (CATTM) behaved as a good cation exchanger with ion exchange capacity of 1.64 meq g-1 for Na+ ions. The sequence of ion exchange capacity for alkali metal ions was found to be K+> Na+> Li+ and that for alkaline earth metal ions was Ba2+ > Ca2+ > Mg2+These orders revealed that the ions with smaller hydrated radii acquired larger ion exchange capacity. The pH titration curve indicated that the material obtained as such is a bi functional strong cation exchanger as indicated by a low pH (~2.25) of the solution when no OH- ion was added. Thermal analysis of the material showed that the material retained 55 % of its ion exchange capacity up to 600°C. Adsorption behavior of metal ions in different solvents with varying concentration has also been explored and the sorption studies revealed that the material was selective for Cr(III) and Pb(II) ions. The analytical utility of the material was investigated by performing binary separations of selected metal ions in a column based on the distribution coefficients of the metals. Cr(III) and Pb(II) were selectively removed from synthetic mixtures of Cr(III)-Co(II), Cr(III)-Cd(II), Pb(II)-Co(II) and Pb(II)-Cd(II). Antimicrobial activity of the synthesized titanium (IV) tungstomolybdate compound was evaluated and showed a considerable antibacterial activity against Staphylococcus aureus, Streptococcus agalactiae, Escherichia coli and Shigella flexneri. The inorganic counterpart has also exhibited a promising antifungal activity against Aspergillus niger and Fusarium oxysporum.

Abstract ID: 294
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Nanocomposites
Keywords: Nanocomposites; Nickel (Cobalt)-Zinc ferrites; Magnetic properties

Magnetic properties of (Zn;Ni(Co))Fe2O4/SiO2 nanocomposites

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We report on the magnetic properties of the nanocomposites (Zn;Ni(Co))Fe2O4/SiO2 obtained by various preparation routes. Saturation magnetization (MS), remanent magnetization (MR), squareness (S), coercivity (Hc), magnetic moment per formula unit (nB) and anisotropy constant (K) are very important parameters for a magnetic material to be used in technical applications such as high-density data storage, sensors and microwave devices, and medical applications. The magnetic properties of these nanocomposite systems can be controlled by the chemical composition, the mean size distribution, the shapes, and structure of the nanoparticles and by the nature of the matrix in which they are embedded [1-2]. The shape of the hysteresis loop revealed the dependence of superparamagnetic behavior on the structural properties. The replacement of magnetic Co2+ with zero magnetic moment Zn2+ in Co-ferrites induces a gradual reduction of magnetocrystalline anisotropy and the decrease of magnetic coercivity [2]. The magnetic properties are strongly affected by the sample composition and cation distribution within the ferrite structure. The Ni-rich nanocomposites presented superparamagnetic behavior, while the Ni-poor nanocomposites ferromagnetic behavior [1]. Both MS and HC increase with the degree of crystallinity, crystallite size and annealing temperature.

Key Words: Nanocomposites; Nickel (Cobalt)-Zinc ferrites; Magnetic properties

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Abstract ID: 295

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Hard and Soft Magnetic Materials

Keywords: Magnetoimpedance, Skin depth, Magnetic permeability

Effect of spacer layer on Magnetoimpedance of Electrodeposited composite wires

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The giant magnetoimpedance (GMI) effect has been observed in composite wires that consist of a highly conductive non-magnetic inner core and soft magnetic shell [1]. The magnetoimpedance is proportional to the skin depth, which varies with permeability (μ), conductivity (□) and frequency (□). In this work, we present the effect of spacer layer on GMI is studied experimentally. The electrodeposition of NiFe and Cu deposited on 0.1 mm diameter of Cu wire. The electrodeposition was carried out using, NiSO4.6H2O (0.2M), FeSO4.7H2O (0.025M), H3BO3 (0.4M), NH4Cl (0.28M), and Sodium saccharin (1g/L) bath for NiFe deposition and a current density maintained 20mA/cm.2 For Cu deposition CuSO4.6H2O (0.5M), Sodium saccharin (1.2g/L) used as bath. pH of the solution maintained 1.2 by adding sulphuric acid and Current density maintained 84mA/cm.2 Thickness of the NiFe (Pr) is 2μm and Cu layer thickness is 1.2 μm maintained in all the samples. and Further magnetoimpedance measurements were also carried out by using a IM 3536 impedance analyser.

Figure 1:(a) Magnetoimpedance as a function of field, (b) Magnetoimpedance as a function of frequency.

Fig.1 (a) shows that magnetoimpedance as a function of external DC magnetic field. Single layer of NiFe deposited 2 μm deposited on Cu wire, for this sample observed, 121% of magnetoimpedance at 500kHz (sensitivity 4.6%/Oe), image shows that single peak behavior. Double layers of NiFe and Cu were deposited on Cu wire, magnetoimpedance of this sample decreased to 77% at 600kHz (sensitivity 3.3%/Oe). Double layers of NiFe and NiFe were deposited on Cu wire, MI of this sample observed 136% at 200 kHz (sensitivity 10.4 %/Oe). Tri-layer of NiFe, Cu and NiFe films deposited on Cu wire, MI of this sample increased drastically 309% at 300kHz (sensitivity 16.3%/Oe). It indicated spacer layer effect on magnetoimpedance clearly and sensitivity of the sample also improved good amount.

Abstract ID: 296

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Polymeric composites

Keywords: Cobalt ferrite, Polystyrene, Nano, Biomedical, Sensor

Size-controlled synthesis and properties of mangetic polystyrene/Cobalt Ferrite nanocomposites from Styrofoam

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Metal nanoparticles has received much attention in recent years due to its applications in biomedical, sensor, water purification, etc, [1] these applications depend on the size of the nanoparticles formed. However, it is very difficult to maintain size of the material due to its aggregation. Polymer/metal nano-composites are used to overcome this problem [2]. In this study, we synthesize polystyrene/Cobalt ferrite nano-composites with different weight percentages of Cobalt ferrite. Nanoparticle was first prepared by co-precipitation method. Subsequently, polymer/nano composites were prepared by precipitating waste polystyrene solution on Cobalt ferrite suspension. Thermal, Magnetic and structural properties were studied using TGA, DSC, VSM, DLS and SEM analysis. Particle size distribution was measured by DLS method and found that the hydrodynamic size of Cobalt ferrite is 20 nm whereas, the sizes of polymer/metal composites were found to be ~10 nm. SEM images reveal that polystyrene has flat surface and composites have spherical shape. The saturation magnetization of Cobalt ferrite was 33.4 emu/g. It increases from 1.65 emu/g to 3.93 emu/g as cobalt ferrite content in the composite increases. Physicochemical properties offered by the magnetic nano composites shows that the magnetic nano-composites synthesized are suitable for sensor and biomedical applications.

Abstract ID: 297

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Photonic devices and applications

Keywords: Optical Biosensors, FDTD, Photonic Crystal, Nanocavity.

Design a Nanocavity based Photonic Biosensors for detection of Glucose concentration

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In this paper, we have demonstrated and designed a 2D photonic crystal-based biosensor having three cavity structure. These cavity structures are designed by two-line defect and one nano cavity as a sensing cavity. The refractive index of sensing node is changed to according to analyte refractive index. The sensing cavity can detect glucose concentration. Simulation and analysis have been done in order to detect glucose concentration in normal urine (0–15 mg/dL), urine with 1.25, 5, and 10 gm/dL of glucose concentration by analyzing the shift in resonant peak in wavelength range of 1540–1550 nm. For different glucose concentration the refractive index is different so this sensing cavity detect the change in refractive index. Finite-difference time-domain method has been used to analysis the behavior of design structure. It has been observed from the band structure that for little change in refractive index, there will be a shift in the resonant peak as well as transmitted output power and hence it acts as a sensor. For increase the refractive index the resonant peak shifts towards lower wavelength. This indicates that it is highly sensitive for the change in refractive index.

Abstract ID: 298

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Lithium Ion Batteries

Keywords: Lithium ion batteries, Anode materials, nanomaterials, composite structure

Effect of Porous Carbon–Metal Oxide Nanocomposite Structure for Electrochemical Energy Storage Devices

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Electrochemical energy storage devices have attracted enormous interest due to an accelerating global warming and resource depletion. Among them, lithium ion batteries (LIBs) have various advantages such as high energy density (>150 Wh/kg), excellent cycle stability (>1000 cycles), low toxicity, and low memory effects. In addition, as global market of electric vehicles (EVs) are exploding recently, demands for high-performance (high energy and power density, high retention rate, long cycle life and fast charge ability, etc.) LIBs are rising at the same time. LIBs are composed of four main components including anode, cathode, electrolyte, and separator. Among them, carbon-based anode materials such as carbon nanofiber, graphene, carbon nanotube, and graphite are researched broadly due to their good electrical conductivity and superior electrochemical stability. Furthermore, much efforts for composite structure with high capacity nanomaterials (metal, metal oxide, etc.) has been proceeded to enhance the capacity and retention rate [1-2]. These composite structures could effectively restrain the drastic volume changes of metal or metal oxide and improve the electrical conductivity, which leading to an improved electrochemical performance. Thus, in this study, we used porous carbon framework to obtain homogeneous dispersion of metal oxide nanoparticles and investigated the correlation of structural, electrical properties with their electrochemical performances.

Abstract ID: 299
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Nanocomposites
Keywords: Graphene, Molybdenum disulfide, Biosensor, Cancer

Graphene-MoS2 Based Nano-composite for Cancer Biomarker Detection

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Graphene-based nanocomposites have attracted significant interest in the development of new chemical and biological sensors, due to their ultra-high specific surface area and excellent electron mobility [1]. Various nano-materials have been used to improve the structure of graphene for achieving better electrochemical performance [2]. In this work, we have synthesized graphene oxide (GO) molybdenum disulfide (MoS2) nanocomposite (GO-MoS2) via hydrothermal method, where sodium molybdate, graphene oxide, and L-cysteine were used as starting materials. The structural, morphological and elemental analysis of the synthesized GO-MoS2 nanocomposite were carried out using X-ray diffraction, scanning electron microscopy, transmission electron microscopy and Fourier transform infrared spectroscopy. Further, GO-MoS2 nanocomposite has been electrophoretically deposited on indium tin oxide (ITO) coated glass substrate to fabricate an electrochemical biosensor for the detection of cancer biomarker (EpCAM) by immobilizing anti-EpCAM. The electrochemical response studies of this fabricated immunoelectrode exhibited a wider linear detection range (0.001ng mL-1–60ng mL-1) with a low detection limit (0.001ng mL-1) for detection of the EpCAM antigen. In addition, the fabricated biosensor showed good selectivity, reproducibility and holds great promise for the development of an ultrasensitive biosensor for early detection of cancer biomarkers.

Abstract ID: 300

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Anodes and cathodes Materials

Keywords: Key Words: Li metal battery; In – situ plating; composite layer; wettability; lithophilicity; dendrite suppression

Investigating the comprehensive effect of organic - inorganic composite coating to enhance the cyclability of in – situ plated Li - metal battery

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The realization of lithium metal battery ((LMB) is a promising approach to meet the increasing demand of high energy density battery for portable electronic devices and electric vehicles1. However, the highly reactive nature and uncontrolled growth of Lithium (Li) causes continuous accumulation of solid electrolyte interphase (SEI) on negative electrode resulting low coulombic efficiency and short cycle life with possible explosion risks2. Here we report the comprehensive effect of Polyacrylonitrile (PAN) based composite layer coated on the surface of Cu current collector. The excellent wettability and electrolyte uptaking nature of the composite promotes uniform ionic flux and the corresponding electrochemical kinetics. The composite layer offers a moderate mechanical support to the SEI, while it also provides sufficient strength to suppress the growth of lithium dendrites. The formation of new SEI components as lithated metallic oxide reveals the lithiophilic nature of the composite layer to regulate Li+ flux. The interaction of LiPF6 decomposition products with the composite is also indicated. The polymer component endows the composite flexibility nature, and good affinity to lithium flux due to the presence of heteroatoms. SEM and FIB investigation shows that the coating encourages smoother Li+ deposition. The electrochemical performance test indicates improved retention capacity and coulombic efficiency in Cu||NMC (111) and Cu||Li cells. Cu||NMC (111) cell run at 0.2 mA cm-2 retains 30% after 82 cycles, while Cu||NMC cell retains ~30% after only 52 cycles. The coulombic efficiency of Cu||Li cell run at 1 mA cm-2, 1 mAh cm-2 is increased from 91.87% to 97.81% after 120 cycles when composite layer is applied.

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Abstract ID: 301

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Concrete and cementitious composites

Keywords: Magnesium Phosphate Cement, Bonding Mechanism, Durability, Composite Material, Rapid Repair

Bonding Property and Application of Rapid Repair Magnesium Phosphate Cement for Facade and Bottom Damaged Concrete

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While it is well known that if the peeling of concrete walls of structures last for a long time, the steel bars corrosion, the reduction of mechanical properties and the durability of concrete members may appear, and then the structural safety will be affected. Recent research shows that as a base material of cement, magnesium phosphate has quick hardening speed and good early strength compared with the silicate cement which is formerly used, so the time needed to repair the damaged concrete will be greatly reduced. However, the fineness and activity of magnesium oxide, water to binder ratio, magnesium/phosphorus ratio and fly ash content have a significant correlation with the effect of the bond behavior. Therefore, to analyze its mechanism of action and to determine its optimum composition ratio is a key study for Magnesium Phosphate cement concrete repair agent. In this paper, the mechanics and bonding mechanism of Magnesium Phosphate cement concrete repair agent are analyzed. Through the research on the repair process and the operation process of Magnesium Phosphate cement concrete, the relatively better repair plan is designed from the parameter comparison of the matrix strength, the curing conditions, the interfacial condition and the interface treatment method. Based on the actual engineering application, it is verified that the Magnesium Phosphate cement concrete repair agent has good coagulability and bonding performance. Thus, it can be concluded that the Magnesium Phosphate cement concrete repair agent is suitable for rapid repair of the facade and bottom surface of structures.

Abstract ID: 302
Symposium 4: Functional Composite Materials (FCM)
Poster/Oral Presentation
Topics: Multiscale Modeling in Mechanics and Composite Materials
Keywords: functionally graded, hot mix asphalt, interfacial zone, biphasic, micromechanical

A Functionally Graded Micromechanical Model for Simulating the Interfacial Zone in Hot Mix Asphalt

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Hot mix asphalt (HMA) is a three-phase heterogeneous material composed of bitumen, aggregates and air voids. It is so difficult to predict the global and local mechanical behaviour of HMA due to high complex geometry of the inclusions and viscoelastic characteristics of the matrix which varies as a function of time, temperature and loading rate. The interfacial zone (IZ) is the region where the viscoelastic matrix meets the inclusions surfaces. Several physical, mechanical and chemical actions may occur at the IZ during the process of mixing and compacting of HMA. El Haloui et al. [1] investigated the effect of physical properties of IZ by using a micromechanical model. They used a biphasic heterogeneous viscoelastic model to assess different mechanical behaviors of IZ and concluded that this zone has an average behaviour between elastic aggregate particles and viscoelastic matrix. Actually, there is a transition between these two different behaviors (elastic aggregate and viscoelastic matrix) that can be simulated as a functionally graded material by considering different kinds of transitional functions. At last, a numerical model is represented for simulating this transitional behaviour and the precision of the represented numerical model is verified by using experimental results.

Abstract ID: 303

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster/Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: Photocatalysis, Hydrogen, g-C3N4

Photocatalytic H2 Generation with g-C3N4 and MAl2O4 (M=Ba or Mg)

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Photocatalytic hydrogen generation by graphitic carbon nitride (g-C3N4) and spinel type MAl2O4 (M=Ba or Mg) materials photocatalysts is demonstrated. These are proposed as constituents of a g-C3N4 based heterojunction nanomaterial. The g-C3N4 photocatalysts were produced by a facile calcination synthesis process of either urea or thiourea. The MAl2O4 materials were prepared by combustion synthesis but annealed in air or carbon atmospheres. The characterization of these photocatalysts was done using various methods including X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), Raman Spectroscopy (RS), Brunauer-Emmett-Teller (BET) surface area analysis, Diffuse Reflectance Spectroscopy (DRS), Photoluminescence measurements (PL), and Electrochemical Impedance Spectroscopy (EIS). Their evaluation as photocatalysts in a Hydrogen Evolution Reaction (HER) was carried out under the several irradiation sources including a UV mercury pencil lamp, multiple high-power LEDs (UV-vis range) and visible light LED strips. Triethanolamine (TEOA) was used as the sacrificial agent. A maximum hydrogen generation rate of 97 μmol.h-1.g-1 was achieved using the carbon annealed magnesium aluminate whilst the urea derived carbon nitride had a superior performance to the thiourea derived carbon nitride. The results further pave way to the fabrication and evaluation of new heterojunction nanomaterials using urea derived carbon nitride and carbon annealed spinel type materials that may enhance the overall photocatalytic performance of either constituent material.

Abstract ID: 304

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Functional Magnetic Materials

Keywords: L10, high magnetic anisotropy, doping of oxides

The Effect of TiO2 Volume Fraction on the Microstructure and Magnetic Properties of MnAl Thin Film

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Due to low saturation magnetization, high magnetic anisotropy, the L10 -MnAl alloy are very attractive for potential applications in spintronic devices [1]. The doping of oxide might play an important role in controlling the microstructure of the films. Although, there are some study on the effect of doping of TiO2 materials on L10 FePt and CoPt, there are very few reports on L10 –MnAl. Therefore, the TiO2 doping effects on the microstructure and magnetic properties of MnAl thin films were systematically studied. The MnAl:TiO2 were prepared by co-sputtering of MnAl and TiO2 target. The films were deposited on 50 nm CrRu buffered MgO(100) substrate. The growth temperature was kept constant at TS=300°C while the volume fraction of TiO2 was controlled by changing the RF power. The XRD data revealed that the small fraction of TiO2 deteriorated the degree of chemical ordering of MnAl films. This was consistent with magnetic hysteresis loop of the films indicating a significant change in anisotropy energy. With the increase of TiO2 content, the magnetization was gradually found to decrease, while the out-of-plane coercivity was found to increase at first and then to decrease. On the other hand, there was no significant change in the in-plane coercivity. The maximum out-of-plane coercivity was obtained about 5kOe at 5% TiO2 content. The doping of TiO2 might affect the reduction of grain size which causes the increase in out-of-plane coercivity. The surface roughness of MnAl:TiO2 films was found to increase at first and then decreases with the addition of TiO2.

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Abstract ID: 305

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Concrete and cementitious composites

Keywords: Magnesia Phosphate Cement, Cement Concrete Pavement; Thin Layer Diseases; Durability, Rapid Repair

Properties and Application of Magnesium Phosphate Cement for Rapid Repair of Thin Layer

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Nowadays, the number and severity of cement concrete pavement with thin layer diseases is rising year by year. The thin layer diseases not only affect traffic safety, but also bring more serious damage for cement concrete pavement, if it is not repairing in time. For common pavement repairing, traffic has to be closed and restored after a long time. In addition, the thin layer diseases have higher demands on rapid repair material. This study mainly focuses on the rapid repairing material of the cement concrete pavement. The material of thin layer consists of magnesia phosphate cement made up with magnesium oxide, phosphatic ammonia, fly ash et al. It is concluded that it has many advantages in properties through a serial of experiments. Such as fast setting time, early high strength, well fluidity, well abrasion resistance and well corrosion resistance. In order to overcome the shortcoming of limited initial setting time of magnesia phosphate cement in high temperature, this paper discloses optimum dosage of borax retarder by comparative test. Based on the actual engineering application, it is verified that the magnesium phosphate cement concrete has good mechanical properties and durability. Thus, it can be concluded that the magnesium phosphate cement t is suitable for rapid repair of thin layer.

Abstract ID: 306

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Nano, sensor, dendrite, point contact, gas

Quantum nanosensors

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We propose an innovative concept of selective nanosensor for detection of gases and liquids. The device is based on the formation of dendritic point contacts synthesized electrochemically in the probed medium. The temporal dependence of the point contact electrical resistance measured in dynamic mode exhibits step-like structures reflecting the metastable quantum states of the system whose distribution can be presented in the form of conductance histograms. The shape of these histograms vary selectively depending on the nature of the gas or liquid injected in the electrochemical cell near the point-contact. In this way, the obtained conductance histogram is a unique fingerprint of the probed medium and can thus be used to unambiguously identify it. Selective detection of many gaseous and liquid media is possible with this technique including among them methane and rare gases. This new approach is expected to prove its efficiency in searching quantum fingerprints for various applications of such sensors and stimulate the development of the next generation of highly selective nanodevices.

Abstract ID: 307

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Design and application of composite structures

Keywords: Carbon fiber reinforced polymer, crack, experiment, finite element analysis, load-deflection, shear strengthening

A Study on Shear Strengthening of Reinforced Concrete Beams

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Experimental studies are conducted on a control beam and two shear deficient beams strengthened by carbon fiber reinforced polymer (CFRP) laminates. Numerical studies are carried out with finite element analysis using ANSYS software and the results are compared with those of the experimental results. The results are compared in terms of load-deflection, and loads at first crack and failure point. The load at failure for strengthened beams CFRP-SB1 and CFRP-SB2 increases by around 33% and 50% respectively, while the deflection increases by around 97% and 145% respectively when compared to the control beam.

Abstract ID: 308

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster/Oral Presentation

Topics: Electrical, optical, electrochemical, thermal and mechanical properties of graphene, Mxenes and other two-dimensional materials

Keywords: Edge-enriched MoS2; Thin film; Sputtering; Ellipsometry; Wettability; Electrical resistance; Supercapacitor

Single step large area growth of vertically aligned edge-enriched MoS2 nanoflakes: Structure-property tunability with layer number

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Insights into the fundamentals of structure-property relations are one of the most important key parameters, which can be utilized for tailoring numerous material properties such as electrical, optical, wettable and electrochemical for the photonics, optoelectronics, energy storage, and sensing devices. Herein, we report a controlled single-step, large-area growth of highly crystalline MoS2 nanoflakes consisting of vertically grown edge exposed layers using DC magnetron sputtering technique. To understand a correlation between microstructural and material properties, we have been prepared the MoS2 of varying thickness (~1 nm – 440 nm). A number of standard characterization techniques such as XRD, XRR, FESEM, Raman spectroscopy, TEM, and XPS, which confirm the formation of vertically aligned nanocrystalline MoS2 films of different thicknesses. Surprisingly, the growth is readily achievable on a variety of insulating as well as conducting substrates and the growth mechanism is discussed in detail. Wettability results manifest that the water contact angle could be tuned by varying the layer number as well as the exposed edge sites. We have further made an attempt to augment our prevailing understanding of structure-property relations of MoS2 in order to provide large tunability in the optical as well as electrical properties. Spectroscopic ellipsometry results suggest that the complex refractive index (n and k), dielectric function (Ɛ1 and Ɛ2), and optical bandgap (Eg = 1.35 – 1.88 eV) are highly dependent on MoS2 layer number. The MoS2 electrical resistance was observed in the range of 15 kΩ – 98 MΩ and displayed an inverse relationship with the number of layers. Further, we have carried out the charge storage measurements and found the three-electrode cell capacitance to be 5.48 mF/cm2 at a scan rate of 10 mV/s.

Abstract ID: 309
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Polymeric composites
Keywords: Polyimide, Space Weather, Radiation Damage, Geosynchronous Earth Orbit

Dynamics of electron irradiated polyimides in the absence of reactants

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Polyimides are ubiquitous in the aerospace industry as well as a host of other high-performance applications. Understanding the behavior of these high performance organic polymers in a space-like radiation environment is a key step in designing spacecraft for longer mission lifetimes and for remotely diagnosing and resolving spacecraft anomalies. It has been shown that the electrical conductivity and mechanical properties of the commonly used polyimide poly-(pyromellitic dianhydride-4,40-oxydianiline), commonly known as PMDA-ODA or Kapton-HN®, change significantly after exposure to simulated geosynchronous Earth orbit (GEO) conditions.[1] This work will identify electron irradiation-induced changes to the physical properties of PMDA-ODA as well as identify the underlying chemical changes that lead to these modifications. Corresponding spectroscopic changes in the materials will be presented along with the challenges to remote diagnosis, such as in-vacuum self-annealing.[2] Finally, the behavior of composite polyimides such as Kapton® CR and Kapton® CRC under similar GEO-like conditions and their suitability for spacecraft construction will be explored.

Abstract ID: 311

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster/Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: MoS2 thin films; Pd nanoparticles; Hybrid heteronanostructure; Sputtering; H2 gas sensor

Vertically aligned edge-oriented MoS2 hybrid thin film decorated with Pd nanoparticles for room temperature hydrogen sensor

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In the present work, we report a controlled single-step, large area growth of vertically aligned edge-oriented MoS2 hybrid thin film decorated with Pd nanoparticles (Pd/MoS2) on quartz substrate using DC magnetron sputtering technique for room temperature hydrogen (H2) gas sensing applications. The structural, morphological and chemical characterizations were performed using XRD, Raman, FESEM, TEM, EDX and XPS techniques, which confirm the formation of vertically aligned edge-oriented multilayered MoS2 hybrid thin film decorated with Pd nanoparticles. To fabricate the Pd/MoS2 gas sensor, a patterned deposition of Ag electrode on top of Pd/MoS2 was performed by sputtering through a shadow mask. Hydrogen gas sensing performances together with the sensing mechanism of the proposed Pd/MoS2 thin film sensor under low sensing range (10-500 ppm) were discussed in detail. The proposed Pd/MoS2 hybrid thin film sensor shows superior gas sensing performances, e.g., sensing response of 33.7% and response/recovery times of 16 s/ 38 s towards 500 ppm H2, which may be attributed to the combined effect of factors such as hybrid heteronanostructure with unique morphology, catalytic activity, synergistic effects, and heterojunctions. This study offers the development of low power hydrogen sensor for the Internet of Things (IoT) network with advantages of a facile and scalable fabrication technique, room temperature operation, high sensitivity and selectivity, and good reproducibility and durability.

Abstract ID: 312

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Alloy anodes

Keywords: 3D imaging, Si alloy anode materials, 3D Image analysis

Multiscale Investigation of an Si-Fe Alloy Anode Material for Storage Applications with Improved Aging Performance

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Si based Lithium-based technology plays due to its high theoretical capacity performance an important role for energy storage systems [1]. However, there are still several challenges with respect to Si-based lithium (Li)-ion batteries. Mainly those challenges arise due to the large swelling, pulverization, delamination and Li-transport blockage, which lead to strong aging of the batteries or cells. In this context, new advanced designs of the morphology might provide new possibilities with respect to the functional behavior. A highly promising approach in this respect displays the use of silicon-alloy based anode materials.

Since the microstructure of the material relates to the mechanical, electrical and chemical properties of the material, it has a direct impact on the cell performance. Due to the enhanced complexity of those Si-alloy anode materials, the characterization of the microstructure itself and the study of its morphology is very important. Nevertheless, this is demanding due to the different length scales existing in the complex material mix ranging from micro, down to nm on e.g. Si-particle-level. Therefore, a multi method approach with reliable and efficient image analysis algorithm is necessary to provide conclusive information on the different length scales. Such approach may provide improved design guidelines for the used materials as well as for the cells especially for industrial applications.

Considering the complexity of the anode electrode that contains features ranging from tens of µm up to nm scale, a novel correlative approach is applied in this work. To better understand the aging mechanism, we investigated the structural (morphology and crystalline quality) and chemical evolution of the different phases such as Si particles, graphite, and formation of the solid electrolyte interphase (SEI) layer during the charge/discharge process of the electrode as well as the Li-transport blockage characteristic and its impact on the electrochemical performance of the cell. Therefore, we apply 3D imaging methods like SEM/FEB nano-tomography, micro-Synchrotron tomography, micro-XCT as well as a combination of 2D SEM and STEM/EDX. In order to quantify the obtained imaging data we develop and apply an image analysis workflow.

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Key Words: Si-alloy based anode material, Energy Storage, 3D imaging, 3D image analysis

Abstract ID: 313
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Polymeric composites
Keywords: Composite, membrane, surface engineering

Surface engineering of composite membranes and controlling porosity

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Carbon nanotubes are known to impart outstanding bulk properties to polymeric materials into which they are dispersed. Among the polymeric materials, polysulphones form porous materials when they are cast from solution. Controlling the porosity is a challenge which ultimately determines its varied applications. The incorporation of raw CNTs and also functionalized nanotubes into this polymer matrix induces variations in many parameters one of them being the porosity as shown by Shah1. Similarly Gupta2 showed that functionalized single walled nanotubes also alter the porosity and the resulting separating characteristics of aqueous salt solutions. However, the conventional method of measurement of porosity by capillary porometer where high pressures are required damages if not alter the pore dimensions and shape. Whereas when analysed by small angle neutron scattering (SANS), these composites show interesting pore structure as shown by Mangukiya3 and Nikita4. These studies also highlight that nanotubes form linked channels as reflected in the very high pure water flux reported in our studies as well as in other investigations. Removal of heavy metals like Cr(VI) from waste-water was efficient, the composite membranes showing removal capacities of ~95%. We have shown that using suitable chemistry not only the bulk porosity but also the surface can be engineered5. The pure water flux was 446 LMH for membrane with azide functional multiwalled carbon nanotubes and pore dimensions as small as 7.4 nm. Studies show that incorporation of nanotubes results in enhancement of porosity, flux and thermal stability.

Abstract ID: 314

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Multifunctional composites

Keywords: Multiferroic Materials, ME Properties, MD Properties, Composites, Ferroelectric Material

Functional Composite Materials

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Multiferroic materials have gained a renewed interest in the recent years owing to the observation of useful magnitude of magneto-electric susceptibilities reported for the ferrite-ferroelectric composites. Bilayers and Multilayers of different ferroic compositions exhibit longitudinal as well as transverse magnetoelectric properties due to the applied dc magnetic field 'H'. Current research is being carried out to understand the basic physical processes responsible for the observed giant magnetoelectric (ME) coupling and also to realize possible configurations of the ME devices. Barium strontium titanate (BST), Barium zirconium titanate (BZT) systems are well known for their strong response to the applied DC electric field. This property is very attractive and has been used to develop devices operating in RF and microwave frequency range such as phase shifters, tunable capacitance etc.. Here the compositions of BST and BZT are so selected that they are paraelectric with very high ε and very low tan δ at room temperature. As for as the applicability of the thin films of BST and BZT are concerned the product ''γ = Cp* (electrical tunability) / tan δ" is considered as a figure of merit. It has been observed that the particulate nanocomposites of magnetostrictive phase and piezoelectric phase enhances the linear and quadratic ME coefficients. The measurement of ME properties of different compositions of Ni ,Co, Zn ferrites with BZT, PZT or BST nanocomposites with different proportion gives valuable ME MD coefficient.

Abstract ID: 315

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Magnetism and Magnetic Materials

Keywords: Multiferroic, magnetoelectric coupling, sputtering, magnetic field sensor

Strain mediated magnetoelectric coupling in Ni-Mn-In/PLZT multiferroic heterostructure for MEMS device applications

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Recently, multiferroic heterostructures are gaining popularity for pollution free energy harvesting. The fabrications of rarely studied ferromagnetic shape memory alloys (FSMAs) based multiferroic heterostructures are more fruitful because FSMAs possess large magnetostriction compared to reported ferromagnetic oxides, terfenol-D and metglas in literature. In this report, the Ni-Mn-In/(Pb,La)(Zr,Ti)O3 thin film based multiferroic heterostructure has been fabricated using sputtering. The structural and magnetoelectric coupling characteristics of the fabricated heterostructure have been studied. The polarization vs electric field and magnetization vs magnetic field measurements reveal the co-existence of ferromagnetic and ferroelectric orders in all the fabricated heterostructures. The highest magnetoelectric coupling coefficient of 1.28 V/(cm Oe) has been observed. Such Ni-Mn-In/(Pb,La)(Zr,Ti)O3 based multiferroic heterostructures are appropriate candidate for pollution free energy harvesting and microelectromechanical systems (MEMS) based devices applications.

Abstract ID: 316

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Hard and Soft Magnetic Materials

Keywords: High entropy alloys, Ferromagnetism.

Effect of Cu and Mn on the microstructure and magnetic properties of AlNiCoCu(1-x)FeMnx high entropy alloy

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It is well known that multicomponent amorphous alloys exhibit excellent soft magnetic properties for high frequency applications. Study of physical properties of multicomponent high entropy alloys (HEAs) is a subject of recent interest HEAs are preferentially defined as alloys containing at least five principal elements, each with an atomic percentage between 5 and 35%. HEAs with a fraction of ferro and non-magnetic elements have been found to show very good soft magnetic characteristics. It has been found that addition of Cu to soft magnetic AlNiCoFe results in phase segregation with magnetically hard phase with saturation magnetization of 84 emu/g and coercivity of 162 Oe. On the other hand, anti-ferromagnetic nature of Mn is inhibited in AlNiCoFeMn HEA as Al changes the Fermi level and itinerant electron-spin coupling leading to ferromagnetism. This has been validated by First-principles density functional calculations on electronic and magnetic structures. It is anticipated that the proper ratio of Cu and Mn in AlNiCoFe can provide superior magnetic properties. In the present work we have investigated the microstructure and magnetic properties of AlNiCoCu(1-x)FeMnx synthesized by Arc melting(AM) and Alloying by mechanically activated annealing(AMAA). Our structural investigations show evolution of ordered BCC phase from mixed BCC+FCC phase with increase in Mn concentration. The highest Ms and Hc for AM samples were 96.6 emu/g and 36.4 Oe for x=0.75 & x=1 respectively. For AMAA samples the values were 120.4 emu/g and 72.3 Oe for x=0.5 and 0.25 respectively. A comparative study of microstructure and magnetic properties of bulk and fine particles will be presented.

Abstract ID: 317

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Nano silica, Micro silica, cementitious mortal, optimized mixture design

Assessment of optimized mixture design of characteristics of enhanced cementitious mortar containing nano silica and micro silica

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Nowadays, improvement of mechanical characteristics is one of the main challenges in the industry of cement and concrete materials. The use of supplementary materials such as nano particles as replacement of part of ordinary Portland cement, and also geo-polymers are some of the main subjects in the mentioned field. The nano silica particles contain considerable specifications such as pozolanic characteristic, favorable effects on cavity structure modification and improvement of mechanical characteristics. In the current research, full experimental study has been carried out to examine cementitious mortar specimens containing nano silica, micro silica and also PVA fibers. In this work, optimized mixture design containing mentioned ingredients has been carried to improve the 28 day flexural strength of about 20%, and 28 day compressive strength if about 40%. The compatibility tests also has been carried out and showed suitable results. The mentioned results has been obtained from tests carried out on specimens containing nano silica as the replacement with part of the cement with the percentage between 1 to 10%. The whole conclusion of the current research showed that not only the nano and micro particles enhanced the composite characteristics, but also the obtained product could be used as repairing objects for concrete structures.

Abstract ID: 318

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Concrete and cementitious composites

Keywords: Fly ash, GGBS, Recycled coarse aggregate, alkaline liquid, ambient curing and Geo-polymer RAC

A Study on Geopolymer Recycled Aggregate Concrete as Sustainable Material

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Due to increase in green house gases, creating more concern throughout the world. The quantity of CO2 emission is one of the major causes of global warming. World cement production and construction industry is the second highest source of green house gases next to fossil fuels. Whereas, geopolymer recycled aggregate concrete (RAC) is eco-friendly concrete. Geopolymers are known to be good binders in concrete from many decades, as the CO2 footprint is less compared to conventional concrete (CC). Geo polymer Concrete is made by the combination of alkaline based chemicals such as sodium silicate (Na2OSiO2) and sodium hydroxide (NaOH) along with the combination of alumino-silicate based material such as fly ash and GGBS. The rapid development and destruction in the last two decades has led to the generation of huge volumes of demolition materials landfills, from which one of the material which can be re-used is coarse aggregate which is eco-friendly as it is recyclable. The experimental work is been carried out on partial replacement of recycled coarse aggregate in geo-polymer concrete. Firstly, conducted trail mixes to obtaine mix proportion of M20 to M60 grades of geopolymer concrete using 8M (Molarity) with partial replacement of Recycled Coarse Aggregate (RCA) up to 25%. Secondly casted 3 number of cubes for each grade and cured under ambient curing condition further tested as per the standard codal provisions. Finally, geopolymer recycled aggregate concrete (RAC) results were compared with conventional concrete (CC) target strengths and were encouraging the research with good result for mixes developed.

Abstract ID: 320

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Hard and Soft Magnetic Materials

Keywords: Magnetoimpedance, Skin depth, Magnetic permeability

Effect of spacer layer on magnetoimpedance of NiFe/Cu composite wires

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The giant magnetoimpedance (GMI) effect has been observed in composite wires that consist of a highly conductive non-magnetic inner core and soft magnetic shell [1]. The magnetoimpedance is proportional to the skin depth, which varies with permeability (μ), conductivity (□) and frequency (□). In this work, we present the effect of spacer layer on GMI properties of permalloy (Pr) film. The NiFe and Cu films were electrodeposited on 0.1mm diameter of Cu wire. The electrodeposition was carried out using, NiSO4.6H2O (0.2M), FeSO4.7H2O (0.025M), H3BO3 (0.4M), NH4Cl (0.28M), and Sodium saccharin (1g/L) bath for NiFe deposition and a current density maintained 20mA/cm.2For Cu deposition CuSO4.6H2O (0.5M), Sodium saccharin (1.2g/L) used as bath. pH of the solution maintained 1.2 by adding sulphuric acid and Current density maintained 84mA/cm.2Thickness of the NiFe(Pr) is 2μm and Cu layer thickness is 1.2μm maintained in all the samples.

Figure 1:(a) Magnetoimpedance as a function of field, (b) Magnetoimpedance as a function of frequency.

Magnetoimpedance (MI) as a function of external DC magnetic field of NiFe 2μm thick film deposited on Cu wire (See Fig.1 (a)). A MI of 121% at 500kHz (sensitivity 4.6%/Oe) is observed. The NiFe film sandwiched between Cu film and Cu wire exhibited MI of 77% at 600kHz (sensitivity 3.3%/Oe). Thicker film of NiFe (4 μm) was deposited on Cu wire and MI is observed 136% at 200 kHz (sensitivity 10.4 %/Oe). On the other-hand a Cu sandwiched between two NiFe films and deposited on Cu wire exhibited a remarkable improvement in MI i.e, 309% at 300kHz (sensitivity 16.3%/Oe). From these studies we suggest that spacer layer helps in obtaining GMI values with higher sensitivity. Further the frequency dependence of GMI is also shown in figure 1 (b). Detailed magnetic and MI properties will be discussed along with the related theoretical simulations to understand the role of spacer layer in these composite wires.

Abstract ID: 321
Symposium 4: Functional Composite Materials (FCM)
Poster/Oral Presentation
Topics: Bio-composites
Keywords: AQS, electrochemistry, micelle, A549 human lung cancer cells

Formation and Characterization of Sodium 3-Amino-2-Hydroxy-9,10-Anthraquinone-1-Sulphonate and its Copper(II) and Nickel(II) complexes and their distribution in A549 Human Lung Cancer Cell

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Sodium 3-amino-2-hydroxy-9,10-anthraquinone-1-sulphonate (AQS), an analogue of anthracycline anticancer drug, was prepared by sulphonation of 2-amino-3-hydroxy-9,10-anthraquinone (AQ). The Cu(II) and Ni(II) complexes of AQS were prepared and characterized in order to see whether metal complex formation leads to result better anticancer activity. AQS and its metal complexes were characterized by various experimental and theoretical techniques. The electrochemical behaviors of the molecules were studied in aqueous and non-aqueous solutions. Such redox behaviors are related to their biochemical and biophysical mode of action. Results were compared with earlier findings of related molecules. The molecules were also allowed to interact with different surfactant micelles in order to understand whether they permeate a biological membrane. Different binding parameters like binding constant, partition coefficient, Gibbs free energy for interaction and distribution of the experimental molecules between the bulk aqueous phase and surfactant micelles were estimated. Finally to correlate the physiochemical parameters obtained from the above mentioned studies with the biological efficiency of the experimental molecules, they were treated with A549 human lung cancer cell and analyzed by MTT assay. It was found that the molecules induce apoptosis in A549 human lung cancer cells. The apoptotic pathways were characterized by AO/ EB staining, Hoechst Staining and JC-1staining methods.

Abstract ID: 322

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Ferroelectricity and piezoelectricity

Keywords: Lead free piezoceramics, Crystal structure, Electromechanical properties

Structure-Property Correlation in Environmental friendly Lead-Free (1-x)(Bi0.96La0.04)0.5Na0.5TiO3-(x)(Ba0.90Ca0.10)TiO3 Piezoceramics for Potential Applications

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In recent years, Lead free piezoelectric materials have drawn worldwide attention to the alternative replacement of piezoelectric materials with growing concerns about environmental issues in traditional Lead-based Pb(Zr,Ti)O3 (PZT) piezoelectric materials. In the present work, we synthesized a binary solid solution of (1-x)(Bi0.96La0.04)0.5Na0.5TiO3-(x)(Ba0.90Ca0.10)TiO3 ceramics with compositions $x \leq 0.20$ by Semi–Wet Technique. Crystal structure, surface morphology, ferroelectric, piezoelectric and electromechanical properties were studied systematically. XRD patterns of all the specimens show perovskite phase formation. Rietveld crystal structure refinement using XRD data reveals (i) rhombohedral (R3c) structure for compositions $x \leq 0.08$ (ii) coexisting rhombohedral (R3c) + tetragonal (P4mm) (MPB) structures for the compositions $0.10 \leq x \leq 0.15$ and (iii) tetragonal (P4mm) structure for compositions $0.15 < x \leq 0.20$, at room temperature. Raman spectroscopic studies also confirm above structural analysis. Field emission gun scanning electron micrographs (FE-SEM) indicated decrease in average grain size with decreasing BCT concentration in the solid solution. All the specimens exhibit a well saturated ferroelectric polarization (P)–Electric field (E) loop. The composition with x = 0.12 has the highest value of remnant polarization (Pr =30 μC/cm2) with low coercive field (Ec =27.28 kV/cm). Maximum piezoelectric (d33) and electromechanical coefficient (kp) were obtained for composition x = 0.12 due to the coexistence of rhombohedral and tetragonal crystal structures.

Abstract ID: 323

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Concrete and cementitious composites

Keywords: Composites, Cement Mortar, Microstructure, Micro silica, Nano silica

Microstructure and strength correlation of cement mortar incorporating micro and nano silica

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Cementitious materials made of Portland cement are the composite materials with utmost significance in the construction industry due to their enormous applications. The increasing world population and tremendous technological & industrial advancement leading to massive infrastructure requirement has further increased the demand of cement. The production of cement and fine aggregates is not only highly energy intensive, but also pose a threat to the environment due to release of harmful pollutants including particulates and green house gases (GHGs) such as carbon dioxide responsible for global warming and climate change. Hence, it is a major concern of practicing engineers, researchers and environmentalists to implement new techniques for effective sustainable development. The techniques must involve control and reduction of the GHGs emissions and energy use along with replacement of cement by supplementary cementitious materials (SCMs) that would not only reduce the use of cement, but also would enhance the strength and durability of cementitious materials leading to sustainable construction practices. Pozzolans have attracted the widespread attention with their use as SCMs due to their unique cementitious properties. Nano-silica and micro-silica have gained the utmost attention in recent years due to their technical advantage and sustainability action. In this paper, the effect of partial replacement of cement with commercially available micro silica & nano silica and their combination with optimized content of nano silica on the fresh, hardened, micro structural and durability properties of cement mortar has been studied. Further, statistical models for prediction of the various studied properties at the desired curing ages have been designed. Results reveal that the use of micro silica and nano silica for partial substitution of cement has not only reduced the usage of cement but also improved the fresh, hardened and durability properties due to microstuctural development. Thus, the study reveals the beneficiary use of micro silica and nano silica to improve the microstructure and hence the strength & durability properties of cement mortar in need of sustainable construction practices.

Abstract ID: 324

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Lithium Ion Batteries

Keywords: Cathode materials, Lithium Ion Batteries

Investigation of structural and electrical properties of doped LiMn2O4 synthesized by sol–gel method

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In this present study, we have reported the synthesis of Li-rich Li1.2Mn0.54Ni0.13Co0.13O2 and LiNi0.5Mn1.5O4 by sol–gel method which is used as cathode material in Li-ion batteries (LIBs). X-ray diffraction confirms the crystallisation of synthesised material in the hexagonal layered structure of space group R-3 m and spinel cubic structure with Fd3m space group respectively. Fourier transform infrared spectroscopy confirmed the functional groups. Field-emission scanning electron microscopy equipped with X-ray spectrometer attributed to the morphology and elemental composition of the material. Electric and dielectric properties were investigated in the frequency range of 50 Hz–5 MHz for the temperatures ranging from 313 to 773 K. Conduction mechanism of the cathode material in LIBs was investigated for the grain and grain boundaries in the material. Electric properties of the material were investigated in the framework of impedance, electric modulus and conductivity. The activation energy Ea is calculated for LiNi0.5Mn1.5O4 from the Arrhenius plots and it is found to be 0.3713 eV, which indicates the existence of oxygen vacancy in the material. Nyquist plot showed the non-Debye nature of the material. The important parameters such as Maxwell–Wagner relaxation, hopping mechanism, activation energy, ionic mobility in the material are investigated. The interfacial ion transport mechanism of conductivity is studied using Jonscher’s Power Law.

Abstract ID: 325

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: Sb-Mo(O, S)3 oxy-sulfide; photocatalyst; methylene blue; photodegradation

A new highly efficient Sb-doped Mo(O,S)3 oxy-sulfide photocatalyst for degradation of methylene blue by under visible light illumination

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Metal doped oxy-sulfide semiconductors have narrow band gap values suitable for photocatalytic degradation of organic pollutants under visible light irradiation. Methylene blue dye is among environmentally toxic, carcinogenic and mutagenic organic pollutants. For removal purpose, the Sb-doped Mo(O,S)3 oxy-sulfide nanoplate catalyst with different Sb content was successfully synthesized via facile method. The structural, morphological, chemical composition, optical properties and electrical conductivity of the catalyst were successfully characterized. The photcatalytic performance of Sb-Mo(O,S)3 at different Sb content was investigated for the degradation of methylene blue dye under visible light irradiation using hydrogen peroxide as an effective electron scavenger. The 10% Sb-doped Mo(O,S)3 catalyst was found to be an optimum composition, where it degraded 99.8% of the dye within 60 min illumination time. The photodegradation kinetics follows a pseudo-first-order reaction with a rate constant 7.95□10-2 min-1, which is three-fold higher than that for Sb free Mo(O,S)3 catalyst. The 10% Sb-Mo(O,S)3 catalyst showed excellent activity, enhanced stability and reusability performance, with low charge transfer resistance compared to the Sb free Mo(O,S)3 oxy-sulfide nanoplate catalyst.

Abstract ID: 326

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Concrete and cementitious composites

Keywords: Composites, Cement Mortar, Microstructure, Micro silica, Nano silica

Strength and durability aspects of cement mortar in presence of pozzolans

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Pozzolans are the siliceous and aluminous materials that react chemically in fine powdery form with calcium hydroxide and water, the action termed as pozzolanic activity. Pozzolans are primarily used to improve the performance of cementitious materials in terms of high strength, enhanced durability and sustainability. Both, natural pozzolans and artificial pozzolans are used as SCMs nowadays. The technical advantage lies in the enhanced mechanical properties such as compressive strength, split tensile strength, impact resistance and ductility along with mitigation of harmful reactions in cement matrix leading to reduction in permeability and shrinkage. The sustainability action lies in the reduction in the amount of cement and increased durability of the cementitious materials leading to overall decrease in emission of carbon dioxide. Their application to develop the sustainable and environment friendly cementitious composites with high strength and durability is widely accepted and in use in many countries. The paper presents study of strength, durability and workability of cementitious materials with partial replacement of cement with nano-silica and micro-silica. The results obtained have been discussed for all of the studied properties in terms of effect of rate of content enhancement of micro silica and nano silica as partial substituent for cement, as well as increase in curing age. The results reveal the enhanced microstructure, durability and strength properties of the cement mortar that can be tailored further as per need in construction practices.

Abstract ID: 327

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Non-destructive Inspection Techniques for Composite Materials and Structures

Keywords: Micro-holes, topography, colloidal suspensions

Topography studies of silica micro-holes based on AFM characterization and PMMA particles sedimentation

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The characterization of micro-holes produced by laser ablation is presented. The micro structures are formed on soda-lime glass substrates of 0.160 mm thickness. Their geometries and topographies are characterized using Atomic Force Microscopy (AFM) and the Confocal Laser Scanning Microscopy (CLSM). In addition, given that AFM has limited access to the sidewall especially when the sidewall angle is near or greater than 90 degrees, a new technique to improve the characterization by AFM is employed. In CLSM, colloidal suspensions with polymethyl methacrylate (PMMA) particles are prepared and deposited in the micro-structural hole patterns. The analysis of their distribution inside the micro holes and its relation to the topography of the holes is studied. Image processing is carried out using the Interactive Data Language (IDL) software in conjunction with C language programming in order to calculate the radial distribution function g(r) and density profiles ρ(z), which represent the changes in the topography, and to reconstruct the contour plots of the holes.

Abstract ID: 328

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Transparent Conductors

Keywords: Carrier dynamics

Terahertz spectroscopic evidence of electron-electron interactions in SrVO3 thin films

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In this talk, I present the low energy carrier dynamics of the metallic SrVO3 epitaxial thin films by terahertz (THz) time-domain spectroscopy. Temperature-dependent THz optical and electrical conductivity show high metallic behavior with high carrier concentration. The spectral features of THz conductivity model well with the Drude behavior and provide direct evidence of electron-electron interactions. It is found that electron-electron interactions mainly contribute in the conduction mechanism. Our results provide significant insight on low energy carrier dynamics in the correlated electron system, particularly perovskite-based d1 transition metal oxides.

Abstract ID: 329

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Metamaterials and Materials for THz, Plasmonics and Polaritons

Keywords: Terahertz, Polariton, Strong Coupling

Strong Coupling of Terahertz Fields to Collective Intermolecular Vibrations

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Since the first observation of the strong coupling between an optical microcavity and Frenkel excitons in dye molecules, this field has been increasingly drawing interest, driven by the opportunities for tailoring material properties and chemical processes in molecules [1]. Recently, strong coupling of intra-molecular vibrations to mid-infrared resonators was introduced as a new paradigm [2], in which the creation of vibro-polaritons allows the manipulation of molecular processes occurring at the electronic ground-state, by targeting a specific bond inside the molecules [3]. Here, we take vibrational strong coupling into a new regime: we demonstrate, for the first time, strong coupling of collective vibrations in organic molecule crystallites, occurring at THz frequencies. Unlike previously studies of vibrational strong coupling, here the cavity mode is coupled to inter-molecular vibrations, i.e. an oscillatory motion of the molecules with respect to one another.

In our experiments, we used α-lactose crystallites, which exhibit a sharp absorption peak at 0.53 THz, corresponding to a collective, intermolecular vibration in the molecular crystal. We prepared an α-lactose pellet and placed it inside an "open cavity", formed by two thin gold mirrors deposited on quartz substrates, with one of the mirrors mounted on a translation stage, such that the length of the cavity can be continuously varied. When the cavity length was adjusted such that its optical mode is resonant with the collective vibration in the α-lactose, we observe a clear Rabi-splitting around 0.53 THz, signifying the strong coupling between the collective vibrations in the α-lactose crystallites and the cavity and the formation of two THz vibro-polariton states. By recording the field exiting the cavity in the time-domain, we clearly observe vacuum Rabi-oscillations with a period of ~15psec, corresponding to the reversible, quantum-coherent energy exchange between the molecules and the cavity.

This first observation of strong coupling with THz molecular vibrations take strong light-matter coupling and polaritonic chemistry into a new class of material, including polymers, proteins and other organic materials, in which collective, spatially extended degrees of freedom participate in the dynamics.

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Abstract ID: 330

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Functional Magnetic Materials

Keywords: Ferromagnetic layer, piezoelectric layer, magnetoelectric layer

Effect of piezoelectric and ferromagnetic layer thickness of magnetoelectric layer.

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This paper reports the effect of thickness of piezoelectric and ferromagnetic layer thickness in overall magneto-electric efficiency of the bi-layered structured structure. The response ids found is to be maximum when the thickness of the ferromagnetic layer and piezoelectric layers was of similar thickness.

Abstract ID: 331
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Green Composites
Keywords: Chlorophyll, Ethanol, Magnesium Porphyrin, Organic Transistor, Sensor

Leaf extract as Ethanol Sensing Layer in Organic transistors

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The best sensing materials with high selectivity are found in nature. In this work, we use Chlorophyll extracted from Spinach (Spinacia Oleracea) leaves to sense ethanol. Chlorophyll is a form of Magnesium porphyrin that is efficient in detecting ethanol. Chlorophyll has a phytol functional group that may help in forming self-assembled monolayers that forms a good interface with silicon dioxide [1]. A nanocomposite of Poly(3-hexylthiophene) (P3HT) with chlorophyll is prepared and spin-coated on top silicon/silicon dioxide substrates that are patterned with gold inter-digitated electrodes (IDEs) by optical lithography. The P3HT and chlorophyll nanocomposite thin film perform as both the semiconducting layer and sensing layer. A systematic optical study with UV-Visible (UV-Vis) spectroscopy shows the effect of ethanol in the solution phase. The current-voltage characteristics of the transistors help us detect the ethanol in the vapor phase. This method provides a natural green route for ethanol detection. These sensors may be used by food and beverage industry for ethanol content as well as for electronic nose applications.

Abstract ID: 332

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: Cerium oxide, Thin films, Energy applications

Role of dopant cations on functional properties in cerium oxide thin films for energy applications

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Functional properties caused by mobile oxygen ions in solid oxide materials are gaining greater and greater importance for a wide range of applications, such as catalysts, gas sensors, memristors, electrochemical energy storage/conversion systems, including solid oxide photoelectrochemical and fuel cells. New possibilities in thin film fabrication allow the growth of oxide thin films with a more precise control of the structure and chemical stoichiometry, unveiling new perspectives in the study of technologically important properties of oxide materials. While this approach is quite established in the field of nanoelectronics, it has been more recently adopted also to study ion conducting materials, raising the question of whether by using epitaxial thin films the functionalities based on mobile oxygen ions can be properly tuned. In this context, doped ceria is widely investigated for the intricate interrelationship between microstructure and chemical substitution defects affecting the transport and catalytic properties, as well as the photoactive properties exploting the mixed ionic-electronic conductivity and good surface reactivity. We will discuss the results on the epitaxial doped ceria films obtained by complementary state-of-art experimental techniques, both in laboratory and with synchrotron radiation facilities. The amount of doping and the different ion radius size of the rare-earth dopants affect the local structure and defects distribution, which in turn modifies the electronic band structure. We show how such microscopic properties influence ion conductivity, oxygen exchange surface reaction and charge carriers trapped by oxygen vacancies, with particular regard to the doped ceria used in environmental-friendly applications, so as in solid oxide photoelectrochemical cells.

Abstract ID: 333

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: P3HT, Nanocomposite, Green Synthesis, Green Technology, Nano, Nanoparticles, Sensing.

Poly (3-hexylthiophene) nano composites with green synthesized nanoparticles for environmental sensing applications

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Integrating nanoparticles and forming organic nanocomposites that would maintain or enhance the conductivity of organic thin film transistors has been a challenge. We develop a Poly (3-hexylthiophene) (P3HT) nano composite with the green synthesized nanoparticles (NPs) for sensing applications. Silver nanoparticles (Ag NPs) were synthesized using plant leaf extract of Neem plant (Azadirachta Indica), a green technology method. These silver nanoparticles were dispersed in P3HT solution made in dichlorobenzene solvent and spin coated on Silicon/Silicon dioxide wafers patterned with gold electrodes.

By systematically tailoring the nanoparticle size one can tune the effective conductivity of P3HT semiconductor. Additionally the silver nanoparticles embedded in P3HT solution are also useful for direct humidity and temperature sensing. This method not only offers a green

route for developing semiconducting nanocomposites but also opens up wide scope for environmental sensing applications.

Key Words: P3HT, Nanocomposite, Green Synthesis, Green Technology, Nano, Nanoparticles, Sensing.

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Abstract ID: 334

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Poly(Styrene), Cellulose Acetate, Characterization of Nano-Films, Ultrasonic technique, SEM, FTIR studies, Physico-chemical studies, Mechanical studies, Compatibility

STUDIES ON SYNTHESIS AND CHARACTERIZATION OF NANO-FILMS OF POLYMER BLENDS OF POLY(STYRENE) AND CELLULOSE ACETATE

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The polymer blends are physical mixtures of structurally different polymers which interact with secondary forces with no covalent bonding have assumed a very important status scientifically and technologically. Blending is the process of mixing together of two or more different polymers or copolymers, similar to compounding. Polymer blends offer property, cost and processing advantages and they have been used in an increasing number of application. As cellulose acetate is thermoplastic molding material and biocompatible and used in many industrial and biotechnical applications. Ultrasonic studies have been done by Ultrasonic technique. Characterization of polymeric blends of Poly(Styrene) (PS) and Cellulose Acetate (CA) by physico-chemical, mechanical, SEM, FTIR studies over a wide range of concentrations and temperatures have been discussed to study the degree of miscibility, interactions between the polymer and solvent and polymer compatibility.

Abstract ID: 335

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Bio-composites

Keywords: Zinc Oxide Nanoparticles, Alginate Hydrogel, 3D Printing, Antibacterial, Hydroxyl Radicals

Alginate Based ZnO Nanoparticle Scaffolds for Wound Healing

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Effective treatment of chronic wounds is essential for the prevention of infection and scar tissue formation, requiring a novel approach to address the limitations of existing options. This study utilizes calcium chloride (CaCl2) crosslinked alginate, a common biomaterial widely used in wound dressing, and photocatalytically activated Zinc Oxide (ZnO) nanoparticles for their potential hydroxyl radical mediated antibacterial applications. ZnO nanoparticles were synthesized by combustion method from Zinc Nitrate Hexahydrate and Sucrose. SEM and XRD characterization were used to confirm composition and nanoparticle size. Swelling and degradation assays, as well as SEM imaging revealed the greater structural integrity of 3D printed lattice structure compared to those manually cast, with an increased porosity having potential to facilitate molecular exchange. Antibacterial testing suggests that both 0.5% and 1% ZnO concentrations have antibacterial properties comparable to commercially available antibiotic erythromycin, while a Live/Dead assay confirmed viability of fibroblasts on the scaffolds. Overall, this study explores and validates the potential to develop a customizable, biocompatible, and antibacterial patch which can be utilized for chronic wound healing.

Abstract ID: 336
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Green Composites
Keywords: Natural fibers, Thermoplastic Polymers, Composites

Effect of Fiber Loading on the Mechanical and Morphological Properties of Pineapple Leaf (PALF) Fibers Reinforced Thermoplastic Polyurethane (TPU) Composites

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Natural fiber composites are good alternatives to synthetic fiber composites. Advantages such as renewability less abrasiveness to equipment, low density, high specific strength and modulus and price competitiveness make natural fibers superior to synthetic fibers. In this study Pineapple Leaf (PALF) Fibers reinforced Thermoplastic Polyurethane (TPU) composites were prepared. Different fiber contents 20, 30 and 40w% were made. Mechanical and morphological properties were tested.

Abstract ID: 337

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Graphene, Fabry-Perot cavity, Absorption, CVD, Radio Frequency Sputtering

Experimental demonstration of absorption enhancement of single layer graphene in optical resonant cavities

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Electric filed enhancement at the center of a Fabry-Perot cavity was exploited for enhancing the absorption of single layer graphene. Large area single layer graphene grown by chemical vapor deposition was embedded in different optical resonant Fabry-Perot cavities with central wavelengths in the Vis, NIR and IR spectral ranges.

Fabry-Perot filters were fabricated by radio frequency sputtering starting from alternate quarter wave thickness layers of a high refractive index (H) and a low refractive index material. Film materials and substrates were chosen according to the selected spectral ranges. A thin MgF2 layer was evaporated onto graphene layers prior to sputtering process to reduce the sputtering induced damage of graphene.

Experimental absorption values were found in very good agreement with those modeled with COMSOL Multiphysics software.

Abstract ID: 338

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Dielectric materials

Keywords: poly(ether imide)s; fluorene groups; polydimethylsiloxne segments; silica; thin films; dielectric properties

Study on dielectric and thermal behavior of fluorene-containing aromatic poly(ether imide) films

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Highly thermostable low-k dielectric films with potential applications as dielectric materials in microelectronic industry were designed and synthesized starting from a bis(ether anhydride) containing bulky fluorene group, 9,9-bis[4-(3,4-dicarboxyphenoxy)phenyl]fluorene dianhydride, and various aromatic diamines. A poly(ether imide)/silica nanocomposite film was obtained using methyltriethoxysilane as precursor of inorganic phase. The chemical structure was confirmed by FTIR and 1H NMR spectroscopy, and the morphology was investigated by scanning electron microscopy. All the films exhibited excellent thermal stability, having the initial decomposition temperature in the range of 500-530°C, and water vapor sorption capacity in the range of 0.929-1.419 wt%. They exhibited low dielectric constant of 1.98-2.86 and low dielectric loss of 0.0037-0.011, at a frequency of 1 Hz and room temperature. The subglass γ- and β-relaxations, primary α-relaxation and conductivity relaxation process were discussed in respect to the chemical structure of the samples.

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Abstract ID: 339

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Transparent Conductors

Keywords: ZnO, thin films, pneumatic spray, Sn doped, transmission, and XRD

Dual effect to improve the electrical properties of transparent zinc oxide thin films

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The principal aim of this study is to reduce considerably the resistivity of the ZnO thin layers, in this order we try firstly to reduce the concentration of excessive oxygen atoms and secondary we have tested a doping by Tin (Sn) incorporation with different atomic percentages (Sn/Zn=0, 1, 3, 5, wt.%). All the Sn doped ZnO (SZO) films were grown by simple, flexible and cost-effective Nitrogen _ Pneumatic Spray Pyrolysis method (NPSP) on glass substrates at a temperature of 400 °C. The micro-structural, optical, morphological and electrical properties of the films were been studied.

The XRD results demonstrate that the SZO films have polycrystalline nature, and exhibit the preferential orientation of (002) plane, on the other hand, when the concentration of Sn is increased, we notice the appearance of a new orientation (101), which leads to a bidirectional growth. The deposited SZO thin films showed an average optical transmittance in the order of 80 %, in the Uv-visible region (200–800 nm). The band gap values oscillated around 3,27 eV. Photoluminescence (PL) emissions of SZO samples had three main peaks: near band edge emission, and the violet emission and the blue–green emission. Surface morphology of the films obtained by scanning electron microscope (SEM) exhibited the change in morphology with increasing the dopant concentration. A minimum electrical resistivity value around of 17 10-3 Ω.cm was obtained for 3% SZO film. SZO films prepared by NPSP method are promising contender for their potential use as transparent window layer and electrodes in solar cells.

Abstract ID: 340

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Electrochemical Supercapacitors

Keywords: polymeric framework, lamellar, linker, charge capacity storage

Cobalt based lamellar polymeric coordinated like-compounds as supercapacitors: linker effect on the enhancement of the charge capacity

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Recently, researches focused towards the use of energy storage devices have been increased as source of renewable energy. Thus, supercapacitors are a promising alternative, because of their high-power density. In this context, lamellar polymeric-coordinated structures have attracted great research interest due to their extraordinary properties such as fascinating construction. Two Co based lamellar polymeric like compounds were synthesized under vacuum and temperature with different linkers, water and pyrazine (Co-W and Co-P), which act as pillars between the layers formed by Co and terephthalic acid.

Physicochemical characterization was carried out by XRD, FTIR, thermal analysis. Electrochemical studies were carried out at room temperature in a Multichannel potentiostat−galvanostat, classic three electrode cell, a graphite rod and Hg/HgO (1M NaOH) electrode as counter and reference electrode, respectively. The working electrodes were prepared by mixing Co-X materials, amorphous carbon, PTFE binder and ethanol. Onto stainless steel grids, the mixture was compressed and dried.

From XRD and infrared results was confirmed the presence of lamellar structure, showing typical peaks and bands associated to the polymeric coordinated framework.

Electrochemical techniques, Cyclic voltammetry (CV), Electrochemical Impedance Spectroscopy (EIS), Step Potential Electrochemical Spectroscopy (SPECS) and Galvanostatic Charge-Discharge curves (GCD) were employed to examine electrochemical and energy storage properties. The formation of two redox processes was observed for both materials, producing higher currents when pyrazine is present. The faradaic processes observed in both Co X materials, could be attributed to Co2+/Co3+ redox couple with two different cobalt sites due to the dissimilar coordination of cobalt ion to the ligand, the processes are associated to diffusional a non-diffusional control effect. Energy storage processes are detected in the whole potential window, indicating the insertion and extraction of species from solution. From charge and discharge curves of electrodes at different current densities for Co-W and Co-P electrodes, the results exhibited that for all current densities, Co P showed the larger capacity: 80 Cg-1. This fact should be attributed to the stronger Co-Co interaction produced by pyrazine as linker.

Abstract ID: 341

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Sandwich materials/hybrids, Multifunctional composite, Advanced composites

Keywords: Graphene Oxide, Doxorubicin, Enzymatic release, Divinylsulfone

Chemical Activation of Graphene Oxide before Drug Attachment

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Graphene oxide (GO), due to its properties, such as nanometric dimensions, large specific surface area, and good biocompatibility, was used as a carrier in controlled drug release systems. The procedure of its chemical activation before drug molecules binding was elaborated. Graphene oxide solution (1% GO in H2O) was obtained from Graphene Laboratory of the Center of Advanced Studies Warsaw University of Technology (Poland). The particle diameter measured using a particle analyzer (Shimadzu, Japan) was in range 1-5 μm at median diameter of 2.121 mm.

Doxorubicin (DOX), an anticancer drug, was attached to the surface of GO via the Gly-Gly-Leu linker. Hydroxyl groups of GO were activated by 10% v/v sulfone. In the next step, the short peptide (Gly-Gly-Leu) as a linker was attached to the divinylsulfone molecule on GO. Reactive alkenyl groups coming from divinylsulfone molecules on GO that were not joined by the peptide were blocked with ethanolamine. In the next step, the carboxyl group of leucine was activated with DCC. After that DOX molecules were attachment in reaction carried out for 24 hours, at 3°C in a shaking (120 RPM) flask. The carrier was washed three times with 0.1M phosphate buffer pH = 8.0 and each time centrifuged at 10,000 RPM for 15 min. followed by removal of the supernatant and finally dried in a vacuum dryer at 50°C and stored at 3°C.

Approximately 3.07.1020 molecules of the tripeptide were attached to 1 gram of GO and subsequently almost the same number of DOX molecules. The bound DOX was effectively released using thermolysin, an enzyme cleaving peptide bonds between Gly and Leu inside the linker structure. The thermolysin, in its native form, was immobilized inside a core-shell carrier. A porous membrane, made of regenerated cellulose (cut-off 6-8 kDa), was used as the shell was responsible for keeping enzyme molecules and GO particles inside the carrier, simultaneously allowed the released drug molecules to diffuse outside. The released mass of DOX in the 12 days experiment carried out with and without the membrane was comparable what verified positively the assumption that the use of the appropriate membrane does not affect the amount of the drug released into the body.

The rate of drug release was expressed as a function of the enzyme concentration and GO mass packing in reaction volume. The whole process can be divided on three stages and the values of kinetic constants for each of them were determined. The proposed core-shell carriers are an original solution that can be used for many different drugs. However, the release kinetics for each drug and enzyme must be determined independently.

Abstract ID: 342
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Bio-composites
Keywords: 3D bioprinting, cellulose nanocrystal, bioink, microextrusion

Cellulose nanocrystal-biopolymer hybrid bioink formulation for high-resolution 3D printing of heterogeneous tissue constructs

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3D bioprinting is an additive manufacturing process which allows precise positioning of bioinks, composed of biomaterials and living cells, to create 3D tissue architectures that imitate natural tissues and organs. It is deemed the future of biomanufacturing with enormous potential impact on fundamental biomedical research, regenerative and personalized medicine. Even though 3D bioprinting technologies are advancing at a rapid pace, major challenges remain. One of which is bioink formulation. Here, we report a series of studies on a hybrid bioink system incorporating a nanomaterial, cellulose nanocrystal (CNC), and biopolymers for the high-resolution and high-speed printing of 3D tissue constructs via microextrusion. CNC is a type of rod-shaped naturally occurring nanoparticles with proven biocompatibility. Our results show that CNC-biopolymer hybrid bioinks possess promising rheological and mechanical characteristics. In particular, their excellent shear-thinning property ensures facile extrusion through a small nozzle, high print fidelity, and protection of encapsulated cells from mechanical stress-induced cell damage. By chemically modifying CNC, we investigated the effects of CNC surface charge on ink rheology and cell behavior. Two structures with well-defined biomimetic geometries were printed - bi-cellular liver lobule-mimicking constructs and layered colorectal tumor models. Cell viability, function, cell-cell interactions, and cell-extracellular matrix (ECM) interactions in the printed 3D structures were studied. Our studies offer a promising route to greatly enhance bioink formulations for printing complex architectures with multiple ECM components and cell types in sufficient resolution to recapitulate biological functions.

Abstract ID: 343

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Solar Cells

Keywords: Solar Energy, Graphene, Indoor, Nano

Silicon goding indoor

Djordje, Milan Jovanovic[1], Tijana Tomasevic-Ilic[1], Milos Petrovic[2], Nikola Tasic[3,4], Marko Spasenovic[5], Konstantinos Rogdakis[2], Lucio Cina[6,7,8], Aleksandar Matkovic[9], Rados Gajic[1], Emmanuel Kymakis[2]

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We develop efficient indoor (low-light) graphene/n-Si Schottky-junction solar cells that have up to 10% efficiency. The cells are produced from liquid phase exfoliated graphene made by Langmuir-Schaefer assembly. Solar cell performances are tested under different light intensities, from indoor to outdoor (0.2-100mW/cm2). Our solar cells perform better in indoor then outdoor light conditions. For illumination of the 0.002 Sun, the solar cells have up to 10% efficiency and just 0.2% for illumination of 1 Sun, which is the 50 times increase in efficiency for indoor condition. The high efficiency under low light is caused by large shunt (parallel) resistance. Our cells are, according to our knowledge, the highest efficiency Schottky-junction solar cells made by LPE 2D materials. Furthermore, we show that in low-light conditions, our cells are more efficient than Schottky-junction solar cells made by monolayer CVD graphene, and a reference c-Si solar cell. Based on a literature search, we conclude that our solar cells are even two times more efficient than commercial solar cells at low light. We also found that our cells are stable for at least 180 days. A good low light performance could significantly extend the usage and value of Si solar cells towards indoor light conditions. Furthermore, the low cost solution production process of the graphene films will have an important impact on faster adoption of these devices.

Abstract ID: 344

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Optical properties and spectroscopy of graphene and other two-dimensional materials

Keywords: MoS2, RE-ion dopant, Photoluminescnce, Optical Nonlinearity

Spectroscopic and Structural Properties of Atomically Thin Yb3+-doped MoS2 films, deposited using near-IR femtosecond pulsed laser source

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The physics of two-dimensional (2D) materials, such as graphene and transition metal dichalcogenides (TMDs) have been investigated for a range of optoelectronic device applications [1]. Tuneability of bandgap and control of photoluminescence wavelength in 2D materials are important features for demonstrating applications in energy conversion, light emission, and spintronic devices [2]. Recently, the 2D layered materials grown by pulsed laser deposition technique have attracted attention for integrated optoelectronics [3].

In this presentation, we report femtosecond pulsed laser deposition of undoped and rare-earth Yb3+-ion doped MoS2 films. The femtosecond laser with a wavelength of 800 nm, a pulse duration of 100 fs and a repetition rate of 1 kHz were used to deposit the layered MoS2 films. Different deposition parameters were used to form few nano meter thick layered structures of MoS2 films. For achieving such a control of film thickness over 1cm2 deposition area, the laser fluence at 3 J/cm2, Ar pressure of 10 mTorr and substrate temperature at 500oC were maintained. The deposited films were characterized by Raman spectroscopy which clearly showed the characteristic of A_1g and E_2g^1 modes. The separation between the two Raman modes is 23 cm-1, which translates it into the 4-6 number of layers. In Yb3+-ion doped MoS2 films, the Raman modes were shifted to higher frequencies, implying the possible effect of Yb3+ doping and/or defects on 2D MoS2 structure. A further confirmation of the number of layers formed and doping were verified using transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS). Nonlinear optical properties of undoped and doped MoS2 films were studied using open aperture Z-scan technique. For Z-scan, 7 ns pulses from the second harmonics of the Nd-YAG laser centered at 532 nm with a repetition rate of 10 Hz were used to excite the sample. In Yb3+-doped films, enhancement in saturable absorption (SA) at room temperature was observed, which is particularly advantageous for applications in nano-photonic devices such as passive modelocking and optical switches. Our results provide important fundamental insight into the nonlinear optical response and are of crucial importance in designing novel multifunctional rare-earth doped 2D materials.

Key Words: MoS2, RE-ion dopant, Photoluminescnce, Optical Nonlinearity

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Abstract ID: 345

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Carbon/Carbon Composites

Keywords: EMI shielding, nanocomposites, processing techniques

EMI shielding of composites beyond reflection: An Evaluation

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EMI shielding of composites beyond reflection: An Evaluation

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Wide spread applications of electrical and electronic devices in civil, defense, medical and other fields has tremendously increased the electromagnetic (EM) radiation all over. This is really a great concern since EM pollution can cause undesirable EM interference with sophisticated electronic devices besides direct threat to human health and information safety. The possible practical technical way to tackle with unwanted EM radiation is by shielding materials. Reflection, absorption and penetration are the three processes for an incident EM wave passing through any material. Shielding is a blockade to the transmission of EM radiation using effective enclosed area essentially consisted with high conductive materials which can reflect and detain the passing of EM radiation. But, this cannot comprehensively decrease or fade out EM radiation additionally the reflected radiations would cause the secondary EM radiation. Consequently, EM shielding by means of reflection is not the ideal solution to eradicate and regulate EM pollution. EM absorption besides structural design of materials can be the conceivable answer. Through EM absorption the EM energy would be converted to other forms energy under the action of EM loss fillers and the incident waves can be attenuated as much as possible inside of the absorber. In this work, comparative analysis of EMI shielding researches due to reflection and absorption on conducting macro-composites and nanocomposites in correlation with reflectance, absorbance, and transmittance has been presented. Various processing techniques reported in literature in preparation of composites for realization of better SE with low content of filler in composites has also been examined.

Key Words: EMI shielding, nanocomposites, processing techniques

Biography

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30+ years-Teaching, Research and Academic administrative experience.

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Principal Investigator UGC Govt of India project on EMI Shielding at Department of Physics and Astrophysics Principal Investgator UGC Govt. of India project on polymer sensors at Department of Electronic Science, University of Delhi South Campus

HES-Associate Professor Government of Haryana

Published numerous research papers in reputed journals, was member of many academic and professional bodies

Abstract ID: 346

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanoparticles, Nanowires, and 3D Structures

Keywords: CdS Q-dots, Semiconductor, Photoluminescence, Faraday rotation

Spectroscopic and Magneto-optic Properties of Tb3+ and Mn2+-doped CdS Q-dots in Silicate Glass for Faraday Rotation

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We demonstrate the control of Q-dot-scale structures of CdS, Mn2+-doped CdS and Tb3+-CdS in a silicate glass for magneto-optical applications. The microstructural properties of Q-dot glasses were characterized by X-Ray diffraction (XRD), Field Emission Transmission Electron Microscopy (FETEM), UV-Visible-NIR spectroscopy and room temperature Photoluminescence (PL) spectroscopic techniques. The FETEM of the CdS QD–glass structure analysis demonstrates that the size distributions of CdS, Mn2+-doped CdS, and Tb3+-doped CdS Q-dots were in the sub 10 nm nm. The size distribution analysis of Q-dots was found to be consistent with the determination of Q-dot size using the line-broadening measurements in XRD and average Bohr radii estimation using the UV-visible spectroscopy. The XRD and FETEM analyses also confirm that the Mn2+-ions dissolve in the hexagonal CdS structure, consequently the estimated values of lattice parameters of hexagonal CdS are smaller than that for undoped CdS Q-dots. Detailed PL spectroscopic analysis, when excited with 380 nm source, demonstrate the characteristic emission in the 560-750 nm for undoped and 500-725 nm for Mn2+-doped Q-dot CdS glasses, respectively. The changes in line-shapes of PL spectra were also investigated as a function of the heat treatment temperature, from which the process of nucleation and growth of Q-dots were also analyzed and the influence on PL spectra were characterized. The magneto-optical Faraday rotation measurements were studied at room temperature with magnetic fields up to 360 mT for all Q-dot containing glass samples. Significantly, we observed a large increase in the value of Verdet constant from 6.2 to 12.0 degree/T-cm in glass samples with Mn2+-doped CdS[1]. The demonstration of large Verdet constant in Q-dot silicate glasses with sub Tesla field paves the path for engineering range magneto-optical devices for photonics, spintronics and sensors applications, in which the polarization of photons may be controlled with low-intensity magnetic field in glass waveguides and optical fibres.

Abstract ID: 347

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Magnonics and magnetoplasmonics

Keywords: Core-shell nanoparticles, Magnetoplasmonic, Biomedical applications

Physical Properties of Core-Shell Magnetoplasmonic Nanoparticles for Biomedical Applications

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The crystalline magnetic cores Fe3O4, Zn-doped Fe3O4 and CoFe2O4 nanoparticles were prepared through the hydrothermal chemical route. As example the synthesis of CoFe2O4 was done in a PPL lined hydrothermal autoclave at an average temperature of 230 oC for 23 hours. The solvents used were ethylene glycol or triethylene glycol. Cobalt (II) and iron (III) acetylacetonates were used as precursors. With the addition of polyvinylpyrrolidone (PVP) [1] with different molecular weights we have succeed to control the sizes and morphologies of the nanoparticles. Similar route were used for all nanoparticles prepared It was shown an increase of the magnetic moment of Zn doped nanoparticles due to preferential substitution of Zn atoms on octahedral sites of Fe atoms.. Transmission electron microscopy measurements shows different tendencies growth depending of the length of the PVP polymer added. It is important to note that the PVP can change the morphology of the particles from spherical, to cubical or rhomboidal. The prepared compounds are single phase. Magnetic measurements performed in an applied magnetic field between -2 T and 2 T, show small hysteresis loops at room temperature in concordance with the particle size shown on the TEM images. Small coercive fields, HC, were found for all prepared samples. The prepared nanoparticles were covered with SiO2. As functionalization was used 3-Aminopropyl)triethoxysilane (APTES), A solution of HAuCl4 was used in order to obtain the shell. The average diameters of the core-shell nanoparticles were found to be between 85 nm and 172 nm. By Surface Enhanced Raman Specroscopy it was foud an increase in the lines intensity when the gold concentration increase. Finnaly by controlling the electrostatic interactions between cationic liposomes, a new class of versatile multifunctional plasmonic magneto-liposomes has been synthesized. The plasmonic properties of the multifunctional nanohybrids were investigated using UV-Vis absorption and SERS. The possible biomedical applications were also studied.

Abstract ID: 348

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Magnetism and Magnetic Materials

Keywords: Mott insulator, spin-orbit coupling, opposite g-factors, iridium oxides

Novel Magnetisms in Mixed 3d-5d Transition-Metal Compounds

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Combining traditional and relativistic Mott insulators is presented here as a promising route to novel magnetic properties. Such materials could for example naturally take the form of the double-perovskite-like structure AB1-xB'xO3 or the ABO3/A'B'O3 heterostructure epitaxy films where B=3d and B'=5d transition-metal elements. The key mechanism is unusual exchange pathways opened by mixed spin-orbit coupling strengths on the 3d and 5d atoms, as demonstrated in our first-principles-based theoretical analyses of experimental data [1-3]. This renders a spin-flop transition from in-plane to out-of-plane alignment of magnetic moments in Sr2IrO4 upon substitution of Mn or Ru for Ir [1]. In Sr3CuIrO6, the alternating placement of Cu and Ir ions turns isotropic antiferromagnetic superexchange between real spins to anisotropic ferromagnetic exchange between low-energy effective spins [2]. The spin-orbit-entangled isospins of the Ir ions have a negative g-factor of g = –3, opposite to the usual g = 2 on the Cu ions, making this spin-1/2 Ising-like ferromagnet surprisingly exhibit magnetic frustration in the uniform magnetic field and behave like a ferrimagnet with an antiferromagnetic Curie-Weiss temperature. This system also features an exotic magnetic-field driven critical point at which one half of the spins are frozen into a complete order and the other half are fully disordered at zero temperature. The response of this new state to transverse exchange perturbation provides a unique way to realize the long-sought pure XY model system [3].

Key Words: Mott insulator, spin-orbit coupling, opposite g-factors

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Abstract ID: 349

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Superconducting and magnetic materials

Keywords: Y2BaCuO5, Flux, a-c sector

Improvement of magnetic properties and flux pinning for YBCO composites bulk

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Synthesis process of a superconductor can act as flux pinning, resulting in dramatic improvement of magnetic properties. Y2BaCuO5 particles can precipitate inside the superconductor, fill up pores, decrease pores, and result in densification of the superconducting microstructure, thereby improving magnetic properties of the superconducting superconductor. The use of additive brought about the control of Y2BaCuO5 particles, therefor improving superconducting magnetic properties. When applying the interior seeding technique, the processing period was reduced by half. The top seeding effect was obtained by placing one seed on the upper surface, leading to magnetic levitation force. In order to improve physical properties of superconducting materials, the interior seeding technique was applied and top seeding effect was obtained by placing one seed layer on the top surface. The shape of the top surface of the YBaCuO superconducting single crystal bulk varies depending on the thickness of the specimen. The a-c sector area ratio grows significantly with increasing thickness. The area ratio of the a-c sectors increases but the magnetic flotation of the upper surface decreases. This research was supported by the Korea Electric Power Corporation [Grant number: R16XA01].

Abstract ID: 350

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Dielectric materials

Keywords: Molecular Machines, Dipolar Order, Solid state

Emergent Dipolar Order in Amphidynamic Crystals with Freely Reorienting Polar Linkers

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Crystals of freely reorienting 2,2-difluoro-1,4-bicyclo[2.2.2]octane-dicarboxylate (F2 -BODCA) acting as linker and rotator in a metal organic framework (MOF) with Zn(II)-nodes and 1,4-diaza-bicyclo[2.2.2]octane (dabco) spacers, revealed emergent order as a result of correlated dipole-dipole interactions. Variable temperature, frequency-dependent dielectric measurements consisting of a relatively sharp, frequency-independent change in capacitance at Tc =100 K occurred when a rapidly rotating, dipole-disordered, paraelectric phase, transformed into an ordered, antiferroelectric phase where dipole moments largely cancel each other. A frequency-dependent Debye-like dynamic crossover was detected when the rotor dynamics become slower than the frequency of the alternating electric field. The dynamic nature of the F2-BODCA rotators was confirmed by NMR spectroscopy and the energetics of the rotational profile elucidated with the help of Density Functional Theory (DFT) calculations. Finally, Monte Carlo simulations on a 2D rotary lattice revealed a ground state with an Ising symmetry and the effects of dipole-lattice and dipole-dipole interactions.

Abstract ID: 351

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Solar Cells

Keywords: Perovskite, Photovoltaics, Defect passivation

Constructive Molecular Interactions for Surface-defect Passivation in Perovskite Photovoltaics

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A major barrier towards high-efficiency metal-halide perovskite photovoltaics is the surface trap-mediated non-radiative charge recombination. The ionic nature of perovskite lattice enables molecular defect passivation via interaction of functional groups with defects. However, a lack of an in-depth understanding of how molecular surface interaction influences the passivation effectiveness is a challenge for a rational molecular design. Here, the chemical environment of a set of small molecules sharing the identical functional groups but with strategically varying chemical structure were investigated, namely theophylline, caffeine, and theobromine, for defect passivation. When N-H and C=O functional groups were in an optimal configuration relative to the defect, hydrogen-bond formation between N-H and I enhanced the primary C=O binding with the antisite Pb defect to maximize surface-defect binding.

Abstract ID: 352

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multi-scale Modeling of Graphene- and Carbon Nanotube-Reinforced Composites

Keywords: Graphene, Nanocomposite, Thermal conductivity, Kapatiza resistance

Predicting the thermal conductivity of graphene-polymer nanocomposites with consideration of interfacial Kapitza resistance and graphene-graphene contact resistance

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In this report, we demonstrate the development of a theoretical model to evaluate the thermal conductivity of graphene-polymer nanocomposites. Due to the extremely thin aspect ratio of graphene fillers, graphene-graphene contact could easily develop and this would introduce a new contact resistance to thermal transport in the graphene- polymer nanocomposites. The effect of this contact resistance has never been considered before. Here we present a new theory of thermal conductivity that includes both interfacial Kapitza resistance (filler-matrix type) and the graphene-graphene contact resistance (filler-filler type). To account for the effect of graphene-graphene contact, we treat the development of filler networks as a statistical process that can be described by Cauchy's cumulative probabilistic function. With it, a new effective medium theory with a percolation threshold, Kapitza resistance, and graphene-graphene contact resistance is presented. We highlight this new theory by comparing it to four sets of latest ex- periments on the conductivity of graphene/epoxy nanocomposites, and demonstrate that both Kapitza resistance and graphene-graphene contact resistance are essential factors, with the latter gaining increasing importance as graphene loading increases. Several other interesting features of the theory, including the issue of percolation phenomenon and the dependence of filler shape, are also addressed.

Abstract ID: 354

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Mechanical and Thermal properties of graphene, Mxenes and other two-dimensional materials

Keywords: Graphene, defective, residual stress, molecular dynamics

The thermal conductivity of two-dimensional defective graphene under residual stress: a molecular dynamics study

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Previous experiments have proved that single-layer graphene (SLG) has excellent thermal conductivity and can be used as a perfect fillings in thermal interface materials. Therefore, it is of paramount significance to examine the thermally conductive mechanism of SLG. The microscopic defects and residual stresses in SLG are the important factors influencing its thermal conductivity. Limited by experimental technology and economic cost, molecular dynamics (MD) simulation method, as an economic and effective research method, can be widely used Thermal conductivity studies of SLG. It is suggested that the choice of molecular potential functions and thermal conductivity calculation approach will have a decisive impact on the thermal conductivity of SLG. The general molecular potential functions (AIREBO, REBO, CVFF, Tersoff, Reaxff) were used to simulate the different SLG' thermal conductivity responses in the three thermal conductivity calculation approaches (equilibrium MD: EMD, non-equilibrium MD: NEMD, reverse non-equilibrium MD: RNEMD). After the comparison with the experimental results, the detailed comments of each scheme are evaluated, and the optimal molecular potential function and computational approach are selected. We then simulated and calculated the thermal conductivity of SLG containing different defects and subjected to external strain. It is found that the single vacancy, double vacancy and Stone-Wales defects both can greatly reduce the thermal conductivity of SLG and the reduction depends strongly on the type of defects and density. In addition, the thermal conductivity of SLG decreases remarkably under tensile strain. While, it is insensitive to compressive strain.

Abstract ID: 355

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: PMMA, Nano, Optical constant, Hot-Probe, Titanium dioxide.

Evaluation of impurities concentration with hot probe method and optical constants of nano structured titanium dioxide embedded polymer thin films

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Electrical and optical characteristics of nano particle embedded polymer thin films significantly differ from those of pure polymers. Therefore, characterization methods for evaluation of nano particle embedded polymer thin film became highly important. A novel approach to the well-known “Hot-Probe” method is applied in present work. The conventional Hot Probe characterization method enables the definition of a semiconductor type, P or N, by identifying the majority charged carriers. According to the Hot Probe technique, one can measure and calculate the majority charged carriers concentration and its dynamic parameters. In the present report evaluation of majority charged carriers concentration of nano sized titanium oxide embedded PMMA polymer is carried out with Hot Probe technique. The polymer samples are prepared with various concentration of nano sized titanium oxide using casting method. Optical constants of these samples are also determined using transmission and reflection curves in wide range of wavelengths.

Abstract ID: 356

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Design and application of composite structures

Keywords: g-C3N4/I3--BiOI, indirect Z-scheme, self-stabilized I3-/I-

Self-Stabilized Indirect Z-scheme g-C3N4/I3-BiOI for High-Efficiently Photocatalytic CH3SH Elimination

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Methyl mercaptan (CH3SH), a volatile gas with an odor of rotten or cooked cabbage, has a high toxicity and corrosive with very low odor detection thresholds around 0.4 ppb/v. CH3SH is widely produced in urban waste, sewage treatment, industry wastes as well as other energy-related activities.The removal of CH3SH through semiconduction-based photocatalytic process, an economical and environment-benign removal technology, has attracted extensive interest. Here, a self-stabilized Z-scheme porous g-C3N4/I3--containing BiOI ultrathin nanosheets (g-C3N4/I3--BiOI) heterojunction photocatalyst with I3-/I- redox mediator was successfully synthesized by a facile solvothermal method coupling with light illumination, which exhibited substantially high visible-light photocatalytic removal of ppm-leveled CH3SH under LED visible light illumination. The g-C3N4/I3--BiOI heterojunction with 10% g-C3N4 showed a dramatically enhanced photocatalytic activity in removal of CH3SH compared with pure BiOI and g-C3N4, due to its effective interfacial charge transfer and separation. The adsorption and photocatalytic oxidation of CH3SH over g-C3N4/I3--BiOI were deeply explored by in situ DRIFTS, and the intermediates and conversion pathways were elucidated and compared. Furthermore, on the basis of reactive species trapping, ESR and Mott-Schottky experiments, it was revealed that the responsible reactive species for catalytic CH3SH composotion were h+, ·O2- and 1O2, thus, the g-C3N4/I3--BiOI heterojunction followed an indirect all-solid state Z-scheme charge transfer mode with self-stabilized I3-/I- pairs as redox mediator, which could accelerate the separation of photo-generated charge and enhance the redox reaction power of charged carriers simultaneously. The present work could provide promising perspectives in purification of odor gas.

Abstract ID: 357

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: Supercapacitor, Lithium ion battery, Hybrid nano-composite material, Supermolecule assembly

Hybrid Nano-composite Material Prepared by Supermolecule Assembly for Supercapacitor and Lithium ion Battery

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Series hybrid nano-composite materials were prepared by supermolecule assembly for supercapacitor and lithium ion battery. For example, In-situ N/S co-doping three-dimensional succulent-like hierarchical carbon [1], porous N, P co-doped reduced graphene oxide promoted [2], carbon dots decorated graphene/polyaniline composites[3], in-situ carbon-coated MnO2 nanosphere[4], 3D sandwiched nanosheet of MoS2/C@RGO[5], carbon nanoparticle-anchored MoS2 nanosheets[6], porous nitrogen-doped reduced graphene oxide[7], carbon nanoparticles anchored graphene nanosheets material[8] by supermolecule self-assembly for supercapacitor. Li4Ti5O12-carbon-reduced graphene oxide microspheres[9], chitosan-confined synthesis of N-doped and carbon-coated Li4Ti5O12 nanoparticles[10] by supermolecule self-assembly for lithium ion battery.

Abstract ID: 358

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Experimental methods for Composite materials

Keywords: Graphene, heavy metal ion, electrochemical sensor, sodium alginate

Detecting heavy metal ions with ultra-low concentrations based on composite material incorporating reduced graphene oxide and sodium alginate

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Heavy metal pollution is one of the most serious environmental problems. The reduced graphene oxide (rGO) with high electron transfer rate is sensitive to some external substance, and can be used to detect heavy metal ions. However, the amount of oxygen-containing functional groups contained in rGO which are used to adsorb metal ions is often not enough to meet the demand of ultra-low concentrations detection. In this study, a method for improving the metal ions detection efficacy via dispersing reduced rGO into alginate hydrogel to form a composite material as an aggregated micro-adsorber was proposed, and the composite gel material was used to detect trace heavy metal ions (Cu2+, Pb2+ and Pd2+) among microelectrodes. In this method, the alginate gel contains a large number of oxygen-containing functional groups which can enhance ions adsorption. In combination with the matched microelectrodes system with a 2 μm electrode gap, the detection of extremely small amounts of heavy metal ion solution with low-concentrations was performed. The results showed that the “gel-graphene” complex could be interpenetrated nanoporous conductive network that can be used to detect these three types of heavy metal ions with ultra-low concentrations, and the curves of volt-ampere (I-V) characteristics measured under different concentrations can be obviously distinguished. The sensitivity of this composite material to detect these 3 types of heavy metal ions is up to 40 ~ 60 dB, which is favorable to the detection of ions with ultra-low concentrations. The minimum limitation of detection concentrations is 1 pM, which is lower than the required inferior limit of ultra-low concentrations in most applications. This study offers a promising way to develop ultrasensitive electrochemical sensor for heavy metal ion detection.

Abstract ID: 359

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Langmuir-Blodgett Films, Phase Coexistence, Phospholipids, Biosensors, AFM

Langmuir-Blodgett Films: State of the Art and Future. Gibb's Phase Coexistence Rule Not Valid at Nanoscale. Nano Biosensor Applications.

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The method to deposit layer-by-layer ordered organic nano thin films on a support from a pre-spread monolayer at the air-water interface developed by Langmuir and Blodgett (LB) received Nobel prize in 1932. At the end of 80s this method became a very hot topic due to hopes that molecular electronics will replace the Si one. The possibility to control the orientation of the molecules, their density and to deposit uniform monolayers with small density of defects, still make this the best method for supramolecular architecture. Modifications of the method like: absorption from subphase; chemical reactions at the air-water interface; nanoparticle and graphene manipulation and deposition, opens new frontiers to the LB method. The most used application is the preparation of the active layer in biosensors. The significant drop in price of the instrumentation and the possibility to study also the monolayer viscoelastic properties helps the spread of this method [1]. For over 30 years we study fluorescently labelled phosphoplipids, which are excellent matrix for biosensor applications, with all existing experimental techniques and computer modeling. Three new effects were discovered, e.g. fluorescence self-quenching in Langmuir films [2] suggested to be used to enhance biosensor sensitivity and selectivity (left figure). The formation of 3D aggregates in the thermodynamic equilibrium below the Equilibrium Spreading Pressure (ESP) [4, right figure] greatly increases reaction surface and thus enhances sensor sensitivity while keeping it very fast. These aggregates are the first experimental evidence that Gibb's phase coexistence rule is not valid at nanoscale [5]. We transduce the biosensor signal with all major techniques: SAW and bulk piezo elements; steady state fluorescence and its kinetics; Electrochemical Impedance Spectroscopy (EIS).

Abstract ID: 360

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Composite structural materials

Keywords: Nanocomposite, MoS2 nanoflakes, Carbon nanoparticles, Photothermal.

Study of Photothermal Heat in MoS2/C Nanocomposite

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Abstract: Since molybdenum disulfide (MoS2) nanoflakes possess unique thermal and optical properties, which are different from their bulk counterparts, they have attracted a lot of attention. In this work, three different samples of MoS2 nanoflakes, carbon nanopaticles and molybdenum disulfide/carbon nanocomposite (MoS2/C) were synthesized by one step hydrothermal method. The structural and optical properties of all samples were characterized by X-ray diffraction (XRD), Transmission electron microscopy (TEM), Raman spectroscopy, Fourier transform infrared (FTIR) and Ultraviolet-Visible (UV-Vis) spectroscopy. These characterizations confirm that carbon nanoparticles are placed between MoS2 nanoflakes successfully. The photothermal results of samples indicate that temperatures of carbon nanoparticles and MoS2 nanoflakes increase with irradiation of 808-nm continuous wave laser. But when composed together, MoS2/C nanocomposite produces higher photothermal heat than each individual sample. Photothermal experiment was also performed for different concentration of MoS2/C nanocomposite liquid solutions. The result shows that the amount of concentration of MoS2/C nanocomposite affects the produced heat.

Abstract ID: 361

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanomaterials and Nanotechnology

Keywords: Transparent amorphous oxide semiconductor (TAOS), Thin films, Indium Tungsten Oxide, Indium oxide, Indium Zinc Oxide, Flexible thin films transistor, Synaptic transistor.

Low Temperature Modulation of Amorphous Metal Oxide Semiconductor for Flexible and Neuromorphic Electronics

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Intensive research interest has observed in the development of Transition Metal Oxides (TMOs) for the wide verities of applications. However, to activate these materials at low temperature become a critical bottleneck to their widespread implementation and compatible with flexible polymer substrates. Low temperature activation can be implemented by changing the cation composition and oxygen vacancy concentration. In this report, we firstly demonstrated and standardized highly controllable activation of several TMO by this unique route at very low temperatures. Here we used four different systems of TMO as sputtered IWO, IZO, In2O3, IGZO, and solution processed IZO. The tuning of oxygen stoichiometry of AMOS has been carried out by using a tetramethyl aluminum (TMA) precursor treatment right after the device fabrication process. Typically, Al has low standard reduction potential $E°Al3+/Al = -1.662$ V and smaller atomic size, which enable a stronger bonding between the abundant oxygen atoms inside the AMOS. At the same time, Al atom is also capable of pulling off some of the weakly bonded oxygen atoms from the non-perfect M-O bonds and forms Al-O bonds. This process leads to a decrease of weakly bonded oxygen density inside the film results activation of the TMO systems at low temperatures. The detailed electrical parameter analyses and in-depth study of stochiometric transformations, monitored via spectroscopic measurements (X-ray photoelectron spectroscopy) provide critical insights into the underlying oxygen-vacancy generation mechanism. Demonstration of low temperature activation promises alternative to conventional high temperature annealing strategies, facilitating facile fabrication of multifunctional electronic circuits and neuromorphic transistors for bioinspired computing.

Abstract ID: 362
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Bio-inspired design of composites
Keywords: Aero-GaN, Hollow Nanoparticles, 3D Nanoarchitecture, Dual Hydrophobic-Hydrophilic Behaviour

Bio-inspired nanomaterials based on GaN

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The modern market requires new multifunctional materials which should be compatible with both electronics and living organisms. In this presentation, we report on novel bio-inspired hybrid nanomaterials based on GaN – the second most important nanoelectronic material [1].

First, we report on fabrication of hollow GaN nanoparticles, their inner surface being covered by an ultrathin film of ZnO:Fe. The hybrid nanoparticles are biocompatible and exhibit both piezoelectric and magnetic properties. They are shown to be taken up by the living endothelial cells and, with the time, to penetrate in the cells which can be subsequently guided in a controlled fashion using applied magnetic fields [2].

Second, we report on a novel bio-inspired 3D nanoarchitecture of GaN, called aero-GaN or Aerogalnite, which represents the first artificial material exhibiting dual hydrophobic-hydrophilic behaviour (see [1] and comments in Physics World: https://physicsworld.com/a/hydrophobic-or-hydrophilic-aero-gallium-nitride-is-both/). The 3D nanoarchitecture is based on GaN micro-tubular structures with nanoscopic thin walls, the inner surface being covered by an ultrathin film of ZnO. The micro-tubular structures are shown to self-organize when interacting with water, forming self-healing waterproof rafts with impressive cargo capabilities [1]. The physical properties of aero-GaN will be presented in the context of prospects for applications in pressure sensors [3], biomedicine, microfluidics and microrobotics. Along with this, we will present experimental data demonstrating that the novel nanomaterial exhibits shielding capabilities against electromagnetic radiation in both the X-band (8-12 GHz) and Terahertz regions [4,5]. The shielding effectiveness in the frequency range from 0.25 to 1.37 THz exceeds 40 dB, thus placing aero-GaN among the best Terahertz shields known today [5].

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Key Words: Aero-GaN, Hollow Nanoparticles, 3D Nanoarchitecture, Dual Hydrophobic-Hydrophilic Behaviour

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Abstract ID: 363
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Polymeric composites
Keywords: Magneto-sensitive elastomers, Magneto-mechanical deformations, Elasticity, Material model, Energy method

Material modelling of magneto-sensitive elastomers

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Magneto-sensitive elastomers (MSEs), also known as magneto-rheological elastomers are polymeric composites belong to a class of field-controllable materials with magnetically switchable properties. They consist of micron-sized magnetisable particles incorporated within an elastomer matrix. In the presence of an external magnetic field, the induced magnetic interactions and the corresponding particle rearrangements change the mechanical properties substantially. Additionally, these rearrangements lead to changes in

the macroscopic shape of the sample, known as the magneto-induced deformation effect. The application of the magnetic field also introduces a mechanical anisotropy with an axis of symmetry along the the field. Thus, in the presence of a magnetic field, we assume MSE as a transversely isotropic material. Based on this hypothesis, we aim to derive an effective material model from the free energy of MSE in the dipole approximation. Here, we would like to present our preliminary results, uniaxial deformations of MSE in the presence of magnetic field and its comparison with phenomenalogical material model.

Abstract ID: 364

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: Graphene-coated metal nanoparticles, Water splitting, Electrocatalysis

Novel scalable preparation of single-layer graphene coated-metal nanoparticles for water splitting

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Graphene-coated metal nanoparticles (NPs) have attracted great attention owing to their unique structural, photochemical and electrochemical properties based on electron communication between graphene and metal NPs. The development of highly efficient and non-precious metal-based electrocatalysts for water splitting comprising hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) is still a big challenge. The hybridization of nitrogen (N)-doped carbon and cost-effective transition metals is a promising approach to produce highly active catalysts for HER and OER. Herein, a highly controllable chemical vapor deposition method is designed for large-scale synthesis of nickel nanoparticle wrapped by single-layer N-doped graphene (Ni@SNG), where silica work as molecule sieve to tactfully assist single-layer graphene growth by depressing diffusion of carbon radicals. The Ni@SNG sample synthesized at 800 oC shows excellent activity for HER in alkaline solution with a low overpotential of 100 mV at 10 mA cm-2, which is close to state-of-the-art Pt/C catalyst. Furthermore, the Ni@SNG catalyst supported on nickel foil is developed as a magnetic adsorption binder-free electrode, which exhibits much improved performance on catalytic activity and stability than common Nafion binder-based electrode. Therefore, magnetism adsorption technique, taking full advantages of magnetic catalysts, will be a greatly promising approach to overcome high electron resistance and poor adhesive stability of polymer binder-based electrodes in actual applications.

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Abstract ID: 365

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Lithium Ion Batteries

Keywords: BATTERY, ENERGY STORAGE, MAGNETIC ANODE

Synthesis of nanosized ferrimagnetic hematite embedded in carbon matrix and its application in energy storage

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Transition metals have emerged as most researched material as it possesses various fascinating properties like variable valences, photoluminescence1. Iron is the most well-known magnetic transition metal having three metal oxides: Fe3O4, Fego and Fe2O3. Among different oxides, Fe3O4 is highly magnetic in nature whereas α-Fe2O3 is antiferromagnetic2. α-Fe2O3 possess various interesting properties like wide band gap, absorption in visible region, fluorescence, corrosion resistant, biocompatibility, low cost which makes it suitable candidate for technological applications. However, due to its antiferromagnetic nature magnetic field assisted potential applications are limited. So, here we synthesized ferrimagnetic hematite coated with carbon using one step solid state combustion synthesis. Particle size calculated from TEM is ~ 20-40 nm. Saturation magnetization of ~ 16 emu/g is achieved due to the broken Fe3+-O- Fe3+ superexchange bonds due to the presence of oxygen vacancies in the structure. In addition, smaller particle size gives rise to the change in the magnetocrystalline anisotropy of the sample. Coercivity of the material is calculated to be 100 Oe. Further SQUID measurements are performed in order to study the magnetic property at different temperature (5 K, 150 K and 300 K). Further, this material is used as the anode material for lithium ion battery. Due to the presence of porous carbon matrix and smaller particle size, both intercalation and conversion are found to be the governing mechanism for lithium ion interaction which result in a high capacity and durable anode for lithium ion battery. A 2-fold enhanced capacity compared to commercial graphite anode is achieved.

Abstract ID: 366

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Anodes and cathodes Materials

Keywords: nano, carbon, silicon, energy storage

Design of Materials for Advanced Energy Storage

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The global electrochemical energy storage market ranging from electric vehicles and personal electronics to physical grid storage and defense applications demands the development of new classes of materials for fabricating high performance batteries and supercapacitors. I will describe innovative approaches for the design and synthesis of nanostructured materials towards enhanced reversible capacity; superior rate performance and cycling stability; superior gravimetric capacitance; and enhanced energy density and power density. Hierarchical three dimensional (3D) graphene-carbon nanotube hybrid materials called pillared graphene nanostructures (PGN) grown by chemical vapor deposition possess ultra large surface area, tunability, mechanical durability and high conductivity which are appealing to diverse energy storage systems. Integration of nanostructured pseudocapacitive metal oxides to such 3D hierarchical templates provides superior electrochemical performance. Among the high performance capacitor systems developed includes MGM (graphene-MWNT-Manganese oxide) and RGM (graphene-MWNT-Ruthenium oxide) hybrid systems. High specific/areal capacitance and extended operational voltage window provides an exceptionally high energy density and power density. Similar three-dimensional templates are transformed into cone-shaped carbon nanotube clusters decorated with amorphous silicon for lithium ion battery anodes (SCCC), by depositing amorphous silicon onto the mesoporous nano-carbon templates via magnetron sputtering. The seamless connection between silicon decorated CNT cones and the graphene substrate facilitates charge transfer and provides a binder-free technique for preparing lithium ion battery anodes. Lithium ion batteries based on the SCCC architecture demonstrated ultra-fast charging, high reversible capacity and excellent cycling stability. Mildly reduced graphene oxide (mrGO) and silica coated Sulfur particles (SCSP) have been developed as new generation cathode materials, forming the basis for Li–S batteries. During cycling, SCSPs fracture and release active material, and mrGO helps to contain the ruptured particles, thereby reducing the polysulfide shuttling effects and improving the cycling stability. In addition, I will describe the use of computerized tomography (CT) scans for physical characterization of batteries. Selected metal oxide (MO2) thin film barrier layers have been developed to further mitigate the polysulfide shuttling effects, and to further enhance the performance and cyclic stability of Li–S batteries. Through analysing the binding energies of Li2Sn adsorbed onto selected MO2 surfaces via density functional theory (DFT) calculations and Molecular dynamics (MD) simulations, we show that the strong Li-O bonds dominate the interactions between Li2Sn and selected MO2 surfaces. Our studies demonstrate that selected MO2 thin film barrier layers could be employed to further enhance Li-S battery performance.

Abstract ID: 367

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Mechanical and Thermal properties of graphene, Mxenes and other two-dimensional materials

Keywords: Graphene, Diamene, Diamond, Nanomechanics, phase transitions

Pressure-induced Formation of a New Ultra-hard 2D Diamond Structure: From Graphene to Diamene

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Here, we explore the elastic properties of supported 2D films of graphene by the use of modulated Å-Indentation, an Atomic Force Microscopy (AFM)-based technique capable of achieving sub-Å indentations depths during force-indentation measurements. We experimentally demonstrate that at room temperature and under localized indentation pressure, a single layer of graphene on top of a carbon interface layer (buffer layer), both epitaxially grown on the Si-face of a SiC(0001) substrate, exhibits transverse stiffness superior to that of CVD bulk diamond, it is resistant to perforation by a diamond indenter and shows a reversible change in electrical conductivity upon indentation. Density functional theory (DFT) calculations indicate that the 1+buffer layer graphene film undergoes a pressure-induced reversible phase transformation to a new ultra-stiff, ultra-hard 2D diamond structure, named diamene, followed by sp2-to-sp3 chemical bond transitions. Furthermore, we find that the formation of ultra-stiff diamene is exclusive of 1+buffer layer epitaxial graphene films grown on SiC(0001), and it is not observed in the buffer layer alone, nor in thicker epitaxial graphene. DFT attributes this behavior to the layer-stacking configuration of the graphene films.

DFT calculations also show that the transition to a 2D diamond structure is facilitated by the presence of the interfacial buffer layer, that strongly interacts with the reactive Si-terminated face of the SiC substrate, and that does not require the presence of adsorbates to stabilize the film surface in contact with the indenter. This finding casts light on the importance of the physics of the interface between graphene layers and the interaction with the substrate in the emergence of the hardening effect. Recent experiments indeed demonstrate the absence of the graphene-diamene transformation in exfoliated graphene films of any thickness on SiO2.

Besides graphene, other 2D materials possess the structural characteristic necessary for sustaining a similar pressure-induced sp2-to-sp3 phase transition. In particular, hexagonal boron nitrite (h-BN) may be converted to a stable cubic phase (c-BN) under pressure. Our most recent Å-indentation experiments demonstrate that 2-layer h-BN flakes, consistently exhibit a transverse elastic modulus almost two times bigger than that of the bare substrate. This stiffening effect is observed only for flakes of thickness between 2 to 5 atomic layers, but not in single- nor multilayer (> 6-layer) h-BN, and thus appears to be related to the conversion of h-BN to c-BN induced by the indentation pressure.

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Abstract ID: 368

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Electromagnetic radiation

Keywords: mobile phone, metamaterials, SAR

Left-handed Composite Metamaterial for EM Absorption Reduction in Human Head for L- and C-Bands

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Concern about radio frequency (RF) exposure to humans increases tremendously due to rapid growth in the use of wireless communication systems. Generally, every wireless device for instance, cell phone emits RF electromagnetic energy to surrounding when uses it. The measure of the rate at which this energy is absorbed by the human body is known as Specific Absorption Rate (SAR). The Federal Communications Commission (FCC) set a safety guideline to ensure the mobile phones do not exceed maximum permissible exposure level which operating in highest possible condition. Hence, the focus here is to maintain the SAR limits by designing metamaterial shield that can be attached in mobile phone. In this paper, the investigation of SAR reduction was carried out by utilising commercially available Computer Simulation Technology (CST) Microwave Studio software. Specific Anthropomorphic Mannequin (SAM) phantom was used in this simulation to measure the SAR value. The head phantom shell model filled is with a liquid substance which represents averaged material properties of a real human head according to the IEEE standards. A hand model also set on the right sight of the human head in this study with a simple cell phone model in cheek position of talk mode. The mobile phone with metamaterial design was tested while operating at its highest power level in all resonance frequency bands and in various phone positions to simulate the way different users typically hold a mobile phone. The initial focus of this paper is to manifest metamaterial design with multi-band resonance frequencies and left-handed characteristics. The preliminary results indicated that, the proposed metamaterial design manifest resonance frequencies at 1.26 and 1.98 GHz (L-Band) and 4.13 and 5.26 GHz (C-Band). Besides that, the type of substrate material parametric study revealed that, the material with highest dielectric constant manifest acceptable resonance frequencies and magnitude values. FR-4, Polyimide and Roger RT-6880 substrate material with dielectric constant of 4.3, 3.5 and 2.2 were analysed in this paper. Furthermore, the investigation also showed that, approximately 30% reduction in SAR value for averaged over 1 gm of tissue volume.

Abstract ID: 369
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Polymeric composites
Keywords: Hardware, debris, Fly ash, ingestion limit, fly fiery.

FLYASH AS ESSENTIAL BUILDING BLOCK FOR THE FUTURE

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The study centered on brick that is made up of nearly 100% flyash. The way is assembled uses system hardware like those used as earth block production lines. The brick block delivered were 27% lighter than mud blocks. The brick blocks made from fly ash has higher compressive quality. Other good attributes of the debris blocks was examined. They include security quality, modules of burst, ingestion limit, starting rate of assimilation and sturdiness. These estimations of these attributes for fly fiery remains blocks are amazing and have surpassed those relating to earth block. In addition, fly powder blocks have been created with rosy shading like dirt block. The new blocks have been given the name fly ash bricks. This research shows the advantages of this sort of blocks over normal traditional mud blocks.

Abstract ID: 370

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Fuel Cells

Keywords: Nafion, ionic liquid, fuel cell, PEMFC

Ionic liquids Nafion-based composite membranes for PEM fuel cells

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The Nafion membrane stands out for its conductivity and stability in the proton exchange membrane fuel cell (PEMFC). However, its conductivity decreases after a water loss, above 80 °C. Because of this, there is a need to develop a modified membrane that can operate at higher temperatures and lower relative humidity [1]. In recent years, ionic liquids (ILs) have been considered an attractive alternative for application in PEMFCs due to its properties such as high ionic conductivity and low vapor pressure. The 3-triethylammonium propane sulfonic (TEA-PS) cation associated with the anion tetrafluoroborate, hydrogen sulfate or trifluoromethanesulfonate leads to the formation of three new protic ionic liquids (ILs) 3-triethylammonium propane sulfonic tetrafluoroborate (TEA-PS.BF4), 3-triethylammonium propane sulfonic hydrogen sulfate (TEA-PS.HSO4) and 3-triethylammonium propane sulfonic trifluoromethanesulfonate (TEA-PS.CF3SO3), respectively. As the TEA-PS cation of the ILs has an SO3H group similarly to the Nafion membrane, its presence should increase the number of sites responsible for the proton transport. These ionic liquids that have the same cation and different anions were used as potential modifiers for the manufacture of composite membranes containing Nafion. Thus, this study aims to investigate the effect of the anion nature of ILs added to a Nafion membrane by using ILs with the same cation and different anion. The composites were investigated by TGA, XRD, water uptake, leaching, conductivity, and fuel cell performance. The results show that the IL addition improves the thermal stability, hydrophilicity, conductivity, and leads to a decrease of oxidative degradation against Fenton's reagent compared to the pristine Nafion. About water uptake, the more hydrophobic the anion, the weaker is its interaction with the solvation water, and the lower the water absorption by the membrane, in the order HSO4- < BF4- < CF3SO3-. About conductivity analyses, the anion, probably makes weaker H-bonds with the -SO3H group of TEA-PS+, which may facilitate self-ionization and increases ionic conductivity. Impedance experiments showed that the composite membranes with 5 wt.% of IL present the highest ionic conductivity when compared with the others. The membranes had their performance evaluated in PEMFCs. The fuel cell performance of Nafion/TEA-PS.HSO4 is superior to that of the pristine membrane either at 80 °C and 100 ºC. The best PEMFC performance of this composite membrane is attributed to the presence of two protonic groups in the TEA-PS.HSO4 IL, (SO3H in the cation and SO4H in the anion) which increase the number of charge carriers due to their dissociation in the presence of water. This work shows that this composite membrane is very promising for PEMFC applications.

Abstract ID: 371

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Electro-thermal properties of composite materials

Keywords: Core-shell fabrication, MWCNT, Aluminum nitride, Thermal conductivity

: Core-shell Fabrication of MWCNT-AlN/Poly(phenylene sulfide) Composite for High Thermal Conductivity With Effect of Electrical Insulation

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Polyphenylene sulfide(PPS) is super-engineering plastic used for various industrial applications due to its outstanding thermal properties. Here we report a PPS composite, which has high thermal conductivity, containing multi walled carbon nanotubes (MWCNT) and Aluminum nitride (AlN) as thermally conductive filler. For using low filler concentration, core-shell fabrication is introduced. Core-shell fabrication is a method that the composite is prepared by the particle coating method into polymer pellets. Melt mixing fabrication needs high filler concentration for high thermal property, whereas the introduced method shows that the consecutive connection of filler particles via the surface of pellets enhances thermal conductivity. In addition, AlN filler on the surface of pellets blocks electron conduction and thus it is possible to apply on electronic components. The results of this study were investigated by FT-IR, SEM, C-therm TCi, TGA, and UTM.

Reference

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Abstract ID: 372

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Manufacturing and formation techniques

Keywords: Thermoelectric, single crystal, GeSbTe, zT

High Thermoelectric Performance of (Ge1-xSbx)Te Single Crystal

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In this work, we report a promising thermoelectric figure of merit zT of 1.8 at 700~740 K was obtained in Sb doped (Ge1-xSbx)Te, x=0.07 crystals grown by the Bridgman method. The substitution of Sb for Ge significantly reduces the excess hole concentration and optimize the carrier which maximize the power factor to 55x10-6 W/cm-K2 with significant Seebeck coefficient enhancement and thermal conductivity but only slightly reduce the electrical conductivity. With the optimized carrier concentration tunning by Sb doping, the Sb doping effectively enhancing the thermoelectric performance of the Sb doping (Ge1-xSbx)Te, x=0.08 to zT=1.8. To understand how the thermal conduction reduction, inelastic neutron scatterings of SIKA for the phonon dispersion relation (PDR) on Γ□ A and Γ □ M energy transfer spectrums was investigated for both specimens. Compared with the pristine GeTe, the significant difference on the G □ M plane and gap-like feature in (Ge0.92Sb0.08)Te revealed that the phonon dispersion is significantly modified after Sb substitution which may explain the thermal conductivity reduction induced by Sb substitution for Ge.

Abstract ID: 373

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Metamaterials and Materials for THz, Plasmonics and Polaritons

Keywords: Graphene, MoS2, plasmon dispersion, plasmon decay, Terahertz

Theoretical comparison of the plasmon dispersion and decay properties of Graphene and MoS2 nanoribbons for THz applications

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Terahertz (THz) gap between the infrared and microwaves has long been an attractive area for many promising applications in several fields, such as the security, wireless communication technology and the spectroscopy fields [1]. Those applications mainly focused on the use of III-V compound semiconductors due to their high electronic properties [2-5], but those materials require expensive and advanced growth setup. In this research, we focus on cheaper alternatives with comparable properties such as Graphene and MoS2. Structures based on these two materials allow the plasma wave phenomena that makes it possible to detect or emit of electromagnetic waves at THz frequencies [6,7]. In this work, the Graphene and MoS2 were patterned into narrow ribbons as a homogenous 2D plane with anisotropic sheet conductivity. A simulation was conducted using the dispersion relation for plasmons in the Graphene/MoS2 nanoribbons array, for both gated and ungated structures. Based on the simulation, the plasmon frequency was found to depend on the angle between plasmon wave vector and the nanoribbons, and the frequency decreased when increasing the angle. The plasmon frequency for ungated MoS2 is about 4.5 THz for $\theta=0^o$, while for the ungated graphene it is about 30 THz for the same angle. On the other hand, the Graphene/MoS2 gated structures have lower plasmon frequency than the ungated structures, which was due to the existence of spacing between the nanoribbons and the gate metal.

The next step will be to add a stub for these nanoribbons structures and to examine experimentally the results of the plasmon frequency at different angles.

Abstract ID: 375

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: Catalysis, Charge Density, Computational Chemistry

New insights in the catalytic activity of cobalt orthophosphate Co3(PO4)2 from charge density analysis

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An extensive characterization of Co3(PO4)2 was performed by topological analysis according to Bader‘s Quantum Theory of Atoms in Molecules from the experimentally and theoretically determined electron density. This study sheds light on the reactivity of cobalt orthophosphate as a solid-state hete¬rogeneous oxidative dehydration and dehydrogenation catalyst. The topological properties identified various faces of the bulk catalyst as possible reactive sites. The charge accumulations and depletions around the two independent five- and six-fold coordinated cobalt atoms, found in the topological analysis, are correlated to the orientation and population of the d orbitals. It is shown that the (011) face has structural features best for catalysis. Five-fold coordinated ions in close proximity to advantageously oriented vacant coordination sites and electron depletions suit the reactant’s oxygen-lone pairs most for chemisorption. This is confirmed both from the multipole refinement as well as from density functional theory calculations. Close-by basic phosphate ions are readily available for C–H activation.

Abstract ID: 376
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Nanocomposites
Keywords: Fusion Energy, Nanostructure, He implantation

Helium management strategy via designer materials: nanochannel W vs He nanochannels

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Helium management strategy via designer materials: nanochannel W vs He nanochannels

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Material degradation due to helium (He) precipitation is a key concern in nuclear energy. This detrimental effect is amplified in fusion plasma facing materials (PFM) due to extremely high flux of He plasma exposure. As a result, the most promising PFM candidate, tungsten (W), has been found to suffer with a bizarre nanostructure formation termed W-fuzz upon He plasma bombardment. Such a hairy W morphology not only significantly reduces the thermal conductivity and surface reflectivity but also endangers core plasma stability once these fragile W fibers break off from the surface. The root cause of the W-fuzz formation is the insolubility of He in virtually all metals and alloys. One of the strategies in managing He effects is to reduce "net" He-flux experienced or "seen" by the material surface through designer nanostructures which can spontaneously release portion of the incoming He particles. Here we present two materials design strategies: engineering open-surface nanochannels in the matrix during the film deposition (nanochannel W) [1] and spontaneously forming He nanochannels in operando through semi-cohesive nanointerfaces in metal multilayers [2, 3]. A variety of characterization tools (RBS, ERD, NRA, PAS, SIMS, SEM, TEM, TDS) are used to measure the film density, surface morphology, He-retention, and He-bubble distributions. Molecular dynamics simulations are performed to help elucidate He-release mechanisms. The performance characteristics of the nanochannel W films (radiation hardening, thermal stability, and fuzz formation) under fusion prototypic conditions will be also reported.

Key Words: Fusion energy, Nanostructure, He-implantation

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Abstract ID: 377
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Smart Composites
Keywords: Zeolitic imidazolate framework-8 (ZIF-8); graphene oxide (GO); composite membranes; organic dyes

Ultrafiltration membrane composites tailored by ZIF@GO with highly improved organic dye rejection performances

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Membrane-based separation technology has attracted great interest in many separation fields due to its advantages of easy-operation, energy-efficiency, easy scale-up, and environmental friendliness Zang et al. (2016). The sufficiency of GO substrates as the main components of the composites to grow nanoscale ZIFs and increase dispersive forces was investigated as a way to control the growth of the ZIFs. These composites were subsequently used for the production of a series of ZIF-8@GO polyethersulfone (PES) composite membranes through a phase inversion method. GO, ZIF-8, ZIF-8@GO and PES membranes incorporated with ZIFs@GO composites were all successfully characterized using a variety of physical-chemical techniques. An increase in hydrophilicity of the composite membranes was observed, which played a significant role in the permeation flux and fouling of the membrane. Addition pathways through the membrane polymer matrix afforded through the porous ZIFs nanomaterials led to decreased tortuosity and hence the observed increased permeate flux in ZIF-8@GO/PES composite membranes compared with pure PES membrane. The nature of the incorporated ZIFs played a positive role in the increased selective rejection ratio observed for organic dyes. Finally, the enhancement in the fouling profile of the membrane composites due to the incorporation of the filler materials was demonstrated. The results showing improvements in membrane performance, i.e. improved water flux, retention ratio, and antifouling performance, demonstrated that using ZIF@GO composite materials as fillers to prepare composite ultrafiltration membranes is a highly efficient and promising way to develop advanced membranes for removal of organic dyes in wastewater.

Abstract ID: 378

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: All solid-state batteries

Keywords: Lithium ion battery, Nanocomposite, All solid state LIB, solid state electrolyte

All-solid-state lithium ion batteries for electric vehicle applications employing silica/ionic liquid nanocomposite electrolytes

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Higher energy storage density, more safety, cost effective, high temperature tolerant as well as long cycle life rechargeable secondary batteries are state-of-the art issues for acceleration of hybrid/electric vehicles and smart grids. Therefore, much efforts have been paid recently for increasing the device's safety issues against such as fire or explosion accidents, that must be solved before the electrical cars become majority over the presently existing combustion engine cars. Among those, All-solid-state lithium batteries are now expected to be a key choice to satisfy both of battery's safety issue and superior electrical energy storage density.

Here, we report a development of quasi-solid- state electrolyte (QSE), for this purpose, which is consisting of nanoparticles and ionic liquid for nanocomposite materials. The novelty of this electrolyte nanomaterials includes that Li ion conducting ionic liquids can be solidified by an interaction with the surface of oxide nanoparticles and therefore, the ionic liquid is connecting nanoparticles to become continuous soft solid matrix. The model of this nanostructures is quite similar to the brick and mortal structure in the architecture which are both flexible and robust. In fact, ionic liquid of 1 mol□L-1 lithium bis(fluorosulfonyl) imide dissolved 1-Ethyl-3-methylimidazolium bis(fluorosulfonyl)imide (LiFSI/EMI-FSI), mixed with 7nm sized SiO2 nanoparticles by 85 vol% turns to a quasi-solid- state electrolyte with transparent, flexible matrix. The solid-state electrolyte exhibited an electrical conductivity of 10.2 mS□cm-1 and self-diffusion coefficient of lithium-containing species as high as 3.3 □ 10-11 m2□s-1 at 35□C. All solid-state Li ion battery devices (Li/QSE/LiFePO4) demonstrated superior charge/discharge cycle performances such as more than 2000 cycles, and rate capability over 5C even under 5 layer stacked 17V-class bipolar laminated device, found to run a test electric vehicle properly.

Abstract ID: 379

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Porous and cellular materials

Keywords: Thermal energy storage, numerical simulation, phase change material, metal foam

Heating and cooling conditions effects on the kinetic of phase change of PCM embedded in metal foam: Experimental and numerical investigations

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Phase change materials (PCM) are attractive candidates for energy storage. They can store large quantities of energy in small volumes at nearly constant temperatures. Despite their advantage, their thermal conductivity is very low with a high-volume change during the melting and solidification process. One way to increase their poor thermal conductivity is to embed them into open cell metallic foams. In this paper, a numerical and experimental study is conducted on the effect of the heating and cooling conditions on phase change kinetics of paraffin embedded in metal foam. A new experimental device has been developed in order to study the phase chage kinetic of PCM embedded in metal foam. Constant heating and sinusoidal heating is similarly investigated. For the constant heat flux, a step function ranging from +1800 W/m2 to -1800 W/m2 is considered, while for the variable heat flux, a sine function having a similar area as step function is considered at one wall of the container to provide heating and cooling of the PCM/ Metal foam composite. A new mathematical model based on the Brinkmann-Forchheimer-extended Darcy equation and the local thermal non-equilibrium model (LTNE) is proposed by applying a two-energy equation. The paraffin phase change is modeled using the enthalpy-porosity method. The numerical results are validated by comparing them with the experimental data. The results showed that at the time of melting it has reduced with sinusoidal heating.

Abstract ID: 380

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Thin Films and Nanomagnets

Keywords: Complex oxide, Nanocomposites, Thin films, Mangetism

Controlling Functional Properties in Oxide Nanocomposite Thin Films via Strain, Defects and Interfaces

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Strain, Defects and Interface play critical role in controlling functional properties in complex oxide heterostructures. These parameters have been extensively studied in controlled synthesis to control physical properties. How to control these parameters in more complex two phase vertical heteroepitaxial nanocomposites and how to use these parameters to tailor functionalities in nanocomposites are much less explored. In this talk, I will first talk about the synthesis of a variety of nanocomposite thin films from a perspective of strain, defect and interface. Nanopillar feature size in these two phase nanocomposites has been found to be a critical parameter to control strain, defects and vertical interface density. In the second part of this talk, I will focus on how the to use these parameters to tune the functional properties such as magnetism, magnetotransport and magnetoelectric coupling.

Abstract ID: 381
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Bio-composites
Keywords: Protein – inorganic hybrids; Anti-cancer activity; Water Purification; Dye degradation; Highly porous BSA-Au hydrogel beads

Protein-inorganic hybrids as anticancer agents and in the purification of water from organic & inorganic pollutants

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Proteins belong to an important and abundant class of natural biomolecules. Usage of such naturally occurring biomolecules for the development of nano-materials not only serve in different applications but would endow its inherent property of immunogenicity, low-toxicity, biocompatibility and easy degradability to the material. Besides all this, these are abundantly available in natural resources. Their nano-structures and thereby the utility can be modified by using relevant metal ions. Therefore, various protein-based materials as hydrogels, beads and nanostructures including surface modified ones have been prepared and explored their applications. Some of those which will be covered in this presentation include, (a) Cytotoxicity of structurally established La3+ complex of apo bovine α-lactalbumin on cancer cells. (b) Injectable, self-healing, and stress sustainable hydrogel of BSA as a functional biocompatible material for controlled drug delivery in cancer cells. (c) Wheat germ agglutinin modified magnetic iron oxide nanocomplex as cell membrane specific receptor target material for killing breast cancer cells. (d) Role of Moringa Oleifera coagulant protein coated copper phosphate nanoflowers for the removal of heavy toxic metal ions and in oxidative degradation of dyes from water. (e) Copper ion-based micro-porous BSA hydrogel in the absorption and degradation organic dyes from water. (f) Highly porous BSA-Au hydrogel beads as smart and pH responsive purification system for selective and efficient removal of organic dyes and heavy toxic metal ions from contaminated water.

Contributions by all the co-workers, critical analysis by the peers, financial support by the funding agencies and the platform provided by IIT Bombay in the past and IIT Tirupati at present are gratefully acknowledged.

Abstract ID: 382
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Industrial applications of composite materials
Keywords: Optimization, metal to plastic conversion, weight reduction, fuel economy, exhaust emissions (pollutants) reduction, Automotive Industry, composites, plastics, sealing systems, hyper-elasticity, friction, rubbing, failure prediction, von Mises stress, con

Converting an under-the-hood aluminum rear retainer to composites for Ford Motor Company

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The automotive industry has been at the forefront of converting traditional metal parts to plastics. The latter surely offer greater design freedom, opportunity for consolidation, fewer assembly operations, reduced secondary finishing, weight reduction, lower total system costs, a range of properties tailored to specific applications, the ability to withstand temperatures, immunity to most chemicals and corrosive environments. They offer processing in many colors, electrical non-conductivity (insulation from electrical shocks), good thermal breaks ("warmth-to-the-touch"), and low sound transmission (tendency to muffle noise). Nonetheless, plastics have only tapped an estimated 15% of their tremendous potential to replace metals. This is particularly to increase with newer high-performance plastics, increasing sophistication in alloying and blending technologies, and use of computer-aided design and engineering (CAD/CAE) systems. The latter enable engineers to visualize complex parts and molding tools more effectively and faster than ever before. This article identifies fundamental steps and requirements to conduct an efficient and successful conversion of metallic parts to plastics, reviewing the replacement design process from concept to production; an under-the-hood rear retainer for Ford Motor Company is detailed as a case study.

Abstract ID: 383

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: Atomic Ag, Water disinfection, Photothermocatalytic, Solar light

Single Ag atom engineered 3D-MnO2 porous hollow microspheres for rapid photothermocatalytic inactivation of E. coli under solar light

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Atomic level Ag loaded MnO2 porous hollow microspheres (Ag/MnO2 PHMs) were prepared by redox precipitation method, and utilized for E. coli inactivation under solar light irradiation. Ag nanoparticles (NPs) can be downsized into single atoms, thereby realizing highly utilization of Ag element as well as achieving superior photothermocatalytic E. coli inactivation for Ag/MnO2 than MnO2 PHMs. Under attack by the optimal 0.3%Ag/MnO2 PHMs with atomic Ag, 7.11 log10 cfu/mL cells can be completely inactivated within 10 min, much faster than the 0.3%Ag/MnO2 PHMs with Ag cluster (3.3 log10 cfu/mL) prepared by photodeposition method, demonstrating the feasibility of redox precipitation to prepare efficient catalyst for water disinfection. Three effects are believed to contribute to this bacterial inactivation enhancement: (1) atomic Ag with high conductivity induces more formation of Mn3+ and oxygen vacancies in MnO2, which can efficiently accelerate the separation of hot electrons and holes generated by MnO2, collectively work with itself generated hot electrons to form into reactive species for photocatalysis; (2) atomic Ag exhibits strong local heating effect and induces higher reducibility for MnO2, considerably enhances the photothermal conversion and lattice oxygen activity of MnO2, thus promoting the thermocatalysis; and (3) the synergism of solar light driven photocatalysis and thermocatalysis through the activated OL. The highly efficient photothermocatalysis make the designed 3D atomic Ag/MnO2 PHMs have a promising antibacterial ability for cleaning the microbial contaminated water environment.

Abstract ID: 384
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Porous and cellular materials
Keywords: Capacitive deionization, carbon nanosheet, hierarchical porous structure, nitrogen/sulfur co-doping

Three-dimensional hierarchical porous heteroatom-doped carbon nanosheets derived from mycelial pellets with enhanced capacitive deionization performance

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To achieve ultrahigh desalination performance for freshwater production, porous carbon materials with high surface area and excellent conductivity have been developed as electrodes for capacitive deionization (CDI). Herein, we synthesized mycelial pellets-derived nitrogen and sulfur heteroatom co-doped three-dimensional (3D) carbon nanosheets (NSHPC) with hierarchical porous structure via a simple strategy by utilizing sustainable mycelial pellets as carbon source, glutaraldehyde as crosslinking agent, zinc chloride as pore forming agent, and thiourea as heteroatom supplier. The as-prepared biomass-derived NSHPC nanosheets with interconnected hierarchical macro-meso-micropores and lamellar structure, exhibits an enhanced electrochemical capacity, with an extremely high desalination capacity of 18.71 mg g-1 in 500 mg L-1 NaCl solution and an excellent cycling stability over 10 cycles. The efficient CDI performance of NSHPC is due to its unique structure, including the 3D network structure formed by bundled nanosheets to provide multi-dimensional ion diffusion pathways and interlayer ion storage, the hierarchical pores to assist efficient ion diffusion and capture, the surface functional group derived from mycelial pellets, and the wettability contributed by the heteroatom co-doping. The design of NSHPC nanosheets provide an essential strategy for rational design of sustainable and cost-efficient electrode materials for CDI technology.

Abstract ID: 385

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Surfactant, Morphology, Silver Nanoparticles, Nucleation.

Effect of Concentration of Green Surfactants on the Morphology of Silver Nanoparticles

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Surfactants or Stabilizing/capping agents play important role in the synthesis of nanoparticles. Degree of agglomeration and shape and size of the nanoparticles can be tuned by varying the concentration of the stabilizing agents/capping agents. In the present work synthesis of silver nanoparticles is done by electrolytic deposition method using silver nitrate as a precursor and onion extract as capping agent. The work focuses on the study of the effect of concentration of the capping agent on the morphology of as-synthesized silver nanoparticles. Various characterization techniques such as XRD, TEM, AFM, UV-visible and PL-spectroscopy are used for the analysis of as-synthesized silver nanoparticles. It was found that mono dispersed spherical silver nanoparticles of smaller size, for higher concentration of capping agent, and poly-dispersed spherical nanoparticles of larger size, for lower concentration of capping agent, were formed. Capping agent at higher concentration encapsulates nanoparticles in the nucleation stage itself inhibiting them to enter into growth stage.

Abstract ID: 386

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: Ti3C2Tx MXene, Mn2+ intercalation, DFT calculations, Microsupercapacitors (MSC), EMI shielding

Cation intercalation into Ti3C2Tx Mxene for enhanced micro energy storage with anti-electromagnetic interference

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Multifunctional and flexible micro power sources featured with high energy have attractive prospect in integrated microelectronics filed in the future. Here, we demonstrate a high capacity electrode material functional with effective anti-electromagnetic interference, Mn2+ ions induced Ti3C2Tx MXene where the strong interaction between cation and surface functional groups (-OH and -O) has a particularly increasing property. By the density functional theory (DFT) calculations, it's innovatively found from simulation that the migrated Mn2+ is tend to be binding with -OH, owing to the orbital hybridization of Mn 3d and O 2p, and the intercalated behavior are generalized as a diffusion-intercalation-binding process. The binding formation provide the enhanced pseudocapacitance and additive interlayer absorption of electromagnetic waves. Thereby, a planar microsupercapacitor (MSC) functional excellent electromagnetic waves shielding performance is successively proposed with the Mn2+ intercalated active materials, exhibiting a high area capacitance of 87 mF cm-2 at 2 mV/s, a remarkable energy density of 48.3 mWh cm-3 and evenly an outstanding electromagnetic interference (EMI) shielding effectiveness (SE) of 44 dB.

Abstract ID: 387

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Graphene, Mxenes and other two-dimensional materials for biomedical and healthcare applications

Keywords: 2D-functional material, chemical moieties, drug delivery

Synthesis of 2D-Nanomatrerials of Graphene Oxide Synthesized by Chemical Reduction Process with Tailoring Surface Chemical Moiety for Biomedical Applications

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A methods has been developed for controlling surface functionality of highly exfoliated 2D-nano graphene oxide (GO) which was synthesized by chemical oxidation of graphite. Raman spectroscopy was applied to identify distinct two peaks of GO and reduced graphene which were further identified with sp2 of carbon atoms of graphitic carbonic by spectroscopy techniques. The characteristic nature of 2D-carbonic materials was confirmed with 1351 cm-1 and 1579 cm-1 peaks corresponding to D and G bands respectively in Raman spectra. XRD were used to quantify Nano-crystallite structures of these materials. Multilayered structures of GO and successive transformation into discrete layers having 200 to 600 nm nano-assemblies of rGO were observed in TEM and AFM analysis. X-ray photoelectron spectroscopy was used to quantify the relative change in percentage proportion of variation in different functionalities of GO synthesized. A relative variation in change in hydroxyl and carboxylic functional groups at the surface at various steps of reducing of GO quantified by X-ray photoelectron spectroscopic. The results confirmed the introduction of oxygen functionalities as -COOH, –OH and C-O-C during synthesis of exfoliated graphene oxide possible in a tunable manner. The GO was further reduced in a controlled way in which multiple steps of different reducing processes applied to achieve a selective reduction of desired functional groups. The results indicates a possibility of tenability in conversion of GO into graphene which was correlated with increased sp2 carbon proportion after selective reduction of the GO. This functionally graded carbonic material further used for n-vitro biocompatibility studies and correlated with surface oxygen functionalities.

Abstract ID: 388

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Solar Cells

Keywords: Neural networks; Algorithm of Levenberg-Marquart; New technique; Optimization; Speed; Precision; Smooth signal; Noise of measurements; Sampling frequency; Pipeline mode; Filtering by slipping average algorithm.

New Intelligent Neural Network Program Developed Based on Revolutionary Predictive Control for a System Tracking

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To increase the power output of a PV module or a field of PV modules, an electronic controller is incorporated between the PV generator and the load, whose role and main objective is the continuous monitoring of the maximum power point of the PV generator commonly known as MPPT (Maximum Power Point Tracking) and this in general per action on a DC-DC conversion device.

The regulation and control techniques provide the impedance matching function, transferring to the load the maximum electrical power output from the PV generator in any the temperature and sunshine conditions.

The development of a revolutionary method based on neural algorithms for the prediction of an instantaneous command is the main objective in our work.

Indeed, the paper presents a new control strategy for the photovoltaic PV, it is a command based on Neuronal Network technique. It is the first time that this technique has been introduced, and proposed by the authors in synthesizing control laws for the converters of electronic power.

The new technical algorithm based on Neural Networks, is designed to be more robust in performance with respect to tracking speed and precision.

Moreover, this new successful technical research, provides a robust neural structure compared to the noisy empirical data used for the prediction of the command. Consequently a smooth control signal without oscillation, targeting exactly the expected optimal control with an independent control of the sampling frequency of the system.

This study, which is followed by a simulation, has enabled us to consolidate the idea that the new Neural Network controller when compared to their classical counterparts, and obtains the best performances concerning the speed of tracking and precision.

The robustness of the networks of neurons opposite the noise of measurements, like, the smoothness of the power signal of PV system generated during the application of the neuronal order, will qualify this command as a practical alternative to the disadvantages recorded on the levels of the classical methods.

Abstract ID: 389

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Dielectric materials

Keywords: Polymer Gate Dielectric, Organic Electronic, Transistor

Low-temperature solution-processed soluble polyimide gate dielectrics: From molecular-level design to electrically stable and flexible organic transistors

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Aromatic soluble polyimides (PIs) have been widely used in organic field-effect transistors (OFETs) as gate dielectric layers due to their promising features such as outstanding chemical resistance, thermal stability, low-temperature processability and mechanical flexibility. However, the molecular structure of soluble PIs on the electrical characteristics of OFETs have not been fully understood yet. In this work, the material, dielectric and electrical properties are evaluated to systematically investigate the chemical structure effect of aromatic dianhydride and diamine monomers on the device performance. Four soluble PIs based on 4,4'-(hexafluoroisopropylidene)diphthalic anhydride (6FDA) and 5-(2,5-dioxotetrahydrofuryl)-3-methyl-3-cyclohexene-1,2-dicarboxylic anhydride, in which monomeric precursors containing different backbones, side groups, and linkages, were employed to compare the chemical structure impact. The dielectric properties, which significantly affect to the charge transport and crystallinity of OSC thin films, clearly depended on the soluble PI types as well as surface energy and thermal stability. Furthermore, the electrical characteristic measurement and parameter extraction of OFETs based on TIPS-pentacene revealed that the 6FDA-based soluble PIs, which lead to high field-effect mobility, near-zero threshold electric-field, and outstanding electrical stability under bias stress, are the most promising gate dielectric candidates. Finally, low-temperature solution-processed OFETs are successfully integrated with ultrathin flexible substrates and they exhibit no significant electrical performance loss after mechanical flexibility tests. This work presents a step forward to the development of soluble PI gate dielectrics for flexible electronic devices with high device performance.

Abstract ID: 390

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanomaterials and Nanotechnology

Keywords: D-Latch, Nanoscaled Single Device, reduced delay, low power

A Noval Nanoscaled Single Device based Transparent Latch

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The rapid growth of integrated circuits (IC) and semiconductor industry in the world is mostly attributed to the scaling of silicon based semiconductor device dimentions. The aaggresive scaling of MOS devices has indeed kept Moore's law valid and alive and is responsible for the realization of IC with billions of transistors. The scaling process includes reducing the device dimensions such as gate length, gate oxide thickness and supply voltage and has enhanced the speed of operation, packing density, functionality etc of IC significantly. The scaling is indeed a backbone of low power consumption in devices. However, the scaling of devices further and further below 22/18 nm technology nodes is extremely difficult due to short channel effects, gate oxide tunnelling, reliability issues etc. The use of various novel device structures has been proposed to address these problems, like FinFET, double gate MOSFET, SiGe FET, carbon nanotube FET (CNTFET) etc. However, the fabrication of such structures is extremly challenging and is a big hurdle in keeping Moore's law valid. One of the promising approches is to go for the nanoscaled multifunctional devices. In multifunctional device concept, gates, blocks and even complete Boolean equation is being realized at the device level; a single transistor realizes inverter, transmission gate, universal gate and even a Boolean equation is being releazed by a couple of transistors. The transistor count is reduced significantly, which results in lower power dissipation enhances speed and functionality. In this work, we propose and simulate a noval multifunction device, which directly releases a D-Latch. The proposed design employs a split double gate metal silicide source/drain Schottky MOS structure. The proposed single device directly realizes the D-Latch action which conventionally is being realized by at least 4 NAND gates, that is, around 16 MOS transistors. The large number of transistors count in the conventional D-Latch nneeds a large space and consumes a large power. Besides, the scaling of transistors degrades the latch performance on account of rise of short channel effects. The novilaty of our design is that a D-Latch gets implemented by a single transistor, which enhances the packing density and reduces the power consumption. One more advantage of the proposed work is the reduced propagation delay which is of the order of 3 ns. Such improved performance parameters of D-Latch will be highly benificial in its implementaion in sequentioal circuits. The mixed mode circuit analysis of the proposed D-Latch has shown a latch action with high logic level (VOH) and low lgic level (VOL) as ~VDD and~ ground respectively and a reasnoable high ION/IOFF ratio.

Abstract ID: 391
Symposium 4: Functional Composite Materials (FCM)
Poster/Oral Presentation
Topics: Industrial applications of composite materials
Keywords: Dyes, Nano-composite, Degradation, solar light, waste water

Synthesis of Al2O3-ZrO2-CuO nano-composities for the treatment of carcinogenic dyes from waste water

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The synthesis, characterization and photocatalytic efficiency of non-traditional Al2O3-ZrO2-CuO-TiO2 nano photo catalysts is reported. The Al2O3-TiO2 support was loaded with different percentage of CuO and ZrO2. A perfect agreement was found between the band gaps of synthesized nano composite measured by UV-Visible diffuse reflectance spectroscopy (DRS) in the solid phase and aqueous medium by UV-Visible spectroscopy. The X-ray diffraction (XRD) analysis showed the composite nature of these catalysts with the preservation of individual uniqueness of each component. The average crystallite size of these composites was found to be in the range of 30 to 50 nm. The Scanning electron microscopy (SEM) analysis confirms the presence of CuO and ZrO2 at the surface of Al2O3-TiO2 support, while Rutherford Back Scattering Spectroscopy (RBS) shows the quantity of the modifiers according to theoretical data. These composites showed an enhanced photocatalytic activity under sunlight for the degradation of dyes..The kinetics of photocatalytic degradation of carcinogenic dyes was evaluated for optimum correlation with the existing models. The stability of the photocatalysts against the photo-corrosion was monitored by analyzing the samples for respective metals in solution after sunlight exposure. In another experiment the efficiency of these composites were also studied under vacuum and high pressure (upto 10 bar). A degradation efficiency of about 99% of these catalysts against dyes was found within only one hour.

Keywords: Dyes, nano-composites, photocatalysis, vacuum, sunlight.
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Abstract ID: 392

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Fiber reinforced Composites

Keywords: CAJRAL; Fibre Metal Laminate (FML); Linear Fickian process; Pseudo-Fickian process; Tensile load bearing capacity.

Experimental investigations on influence of long term immersion of hybrid Fibre Metal Laminate on its physical and tensile properties

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Global warming and climate change have become the talk of the town today. Carbon emission is one of the root causes of these issues. Natural fibres play a vital role in the area of composites and have found wide acceptance in this area. In this work, in a FML (Fibre Metal Laminate) CARAL (Carbon Reinforced Aluminium), a portion of carbon fibre is replaced with jute. The resulting FML is named as CAJRAL (Carbon-Jute Reinforced Aluminium). Since CAJRAL contains jute, a study of its physical and tensile behaviour is required as a result of long term immersion in distilled water for a period of two weeks. Three different stacking arrangements of CAJRAL FML are considered for this study. The effect of water immersion on the tensile load bearing capacities of these laminates is explored. A decrease in the tensile load bearing capacity of these laminates was seen at the end of two weeks. CAJRAL was seen undergoing three different absorption behaviour namely, linear Fickian, pseudo-Fickian and two stage diffusion process.

Abstract ID: 393

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Fiber reinforced Composites

Keywords: CAJRAL and CARAL laminates; damping; natural frequency; cantilever support; fixed support

Influence of jute fibre on the transverse free dynamic responses of carbon reinforced aluminium rectangular plates

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A natural fibre, Jute, is considered in the formation of a Fibre Metal Laminate (FML) for automotive applications. FMLs fabricated with jute namely, Carbon Jute Reinforced Aluminium Laminate (CAJRAL) and without Jute, namely Carbon Reinforced Aluminium Laminate (CARAL) are studied for their dynamic performance. The ability of CARAL and CAJRAL FMLs to bear dynamic loads under fixed and cantilever conditions, along with their modal behavior, are investigated using impulse technique, and are compared. In addition to the above, the damping capability of the CARAL and CAJRAL FMLs are investigated. It is found that, it is beneficial to use CAJRAL in place of CARAL, with respect to the dynamic behavior of FMLs. CAJRAL shows less damping when compared to CARAL FML. The replacement of a portion of carbon with jute in CARAL laminate proves to be highly cost-effective with respect to dynamic performance.

Abstract ID: 394

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Solar Cells
Keywords: Light scattering, Maskless large area, Inverted hemisphere, Multi-textured AZO films, thin film solar cell

Multi-textured AZO films deposited on inverted hemisphere and maskless large area randomly textured glass surface morphologies for silicon thin film solar cells

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We present advanced light scattering schemes using inverted hemisphere and maskless large area randomly textured glass surface morphologies for the enhancement of current density in silicon thin film solar cells. By well controlling the various etching parameters, we were able to prepare the inverted hemisphere and randomly textured glass structures with high transmittance above 90% and variable haze ratio from 20 to 55% in the visible wavelength region. It was observed that haze ratio of textured glass was dependent on feature size, etching depth and rms roughness. Multi-textured aluminum-doped zinc oxide (ZnO:Al) films were deposited on these textured glass structures and showed high transmittance ~85% and haze ratio ~65% in visible wavelength region. Enhancement in haze ratio of multi-textured AZO films was related to an increase of rms roughness as recorded by 3D-alpha step profiler results. Multi-textured AZO films deposited on inverted hemisphere and maskless large area randomly textured glass surface morphologies were employed as a front transparent conductive oxide (TCO) layers for the fabrication of amorphous silicon (a-Si) thin film solar cells (TFSCs). The a-Si TFSCs deposited on inverted hemisphere and randomly textured glass structures showed the short circuit current density of 16.55 and 16.68 mA/cm2 with an efficiency of 9.61 and 9.79%, respectively. We propose these inverted hemisphere and maskless large area randomly textured glass structures with high transmittance and variable haze ratio for future industrial high efficiency Si TFSCs.

Abstract ID: 395

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: Monolayers, Germanene, Silicene, Functionalization, Device

Chemistry of 2D monoelements beyond graphene

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Monoelemental two-dimensional (2D) materials are at the forefront of current material research. Beyond graphene, the large family of unexplored materials remain unexplored. The development of these materials starts rapidly in last few years. In the carbon or so called tetrel group are beyond carbon silicon, germanium and tin. These elements are capable to form a layered allotrope, however the synthesis methods are not so straightforward as for the graphite. All these materials are non-zero band-gap semiconductors with huge application potential in electronic and optoelectronic devices. This property opens new application possibilities in electronic and optoelectronic devices. Also, the research in the field of energy storage and conversion, as well as sensors and other fields, is rapidly growing. The properties strongly correlate with chemical modifications and functionalization. Compare to graphene, the chemistry of its heavier counterparts remains significantly less explored.1

The main rote for top-down methods of synthesis are based on exfoliation and functionalization of Zintl phases with general formula AB2 consisting from hexagonally arranged Si/Ge layers separated by alkaline earth atoms, typically calcium. The exfoliation procedure is typically based on reaction with acid at ow temperature forming hydrogen terminated surface. In this contribution will be demonstrated novel methods and strategies in synthesis and functionalization of silicene and germanene monolayers. The methods providing controlled functionalization surfaces are based on formation of negatively charged silicene/germanene and subsequent reactions with halogenderivatives, formation of reactive halogenated intermediates or direct reactions of Zintl phases with bromine or iodine derivatives. The developed methods were used for introduction of various alkyl and aryl derivatives in order to control transport and optical properties of functionalized materials. The functionalized germanium derivatives exhibit strong photoluminescence, which maxima can be tuned by substitution with various alkyl and aryl derivatives. For newly developed materials were utilized various applications including gas sensors, hybrid organic-inorganic OLED devices and photocatalytic water splitting.

Abstract ID: 396

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Thin Films and Nanomagnets

Keywords: Non-evaporable getter, Ti-Zr-Hf-V film, Secondary electron yield, Vacuum

Properties of TiZrHfV non-evaporable getter films

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The new generation of accelerators places higher requirements on the material of the vacuum chamber surface. Residual gas in the vacuum chamber causes beam loss in the high-energy particle accelerator, which requires minimizing the residual gas in the vacuum chamber to ensure a higher final vacuum. The most direct way to increase the ultimate vacuum is to perform a certain surface treatment on the inner wall to reduce surface outgassing. Therefore, coating a non-evaporable getter (NEG) film on the inner wall surface of the storage ring is an effective method to increase the degree of vacuum. At the same time, the search for NEG materials with low secondary electron yield (SEY) and an effective vacuum chamber surface treatment process can effectively reduce the electron cloud effect, which is an important early work for the new generation of accelerators. In this work, the SEY characteristics of a Ti-Zr-Hf-V NEG film deposited on a Si (111) substrate using a DC magnetron sputtering method are revealed. Surface morphology and surface chemical bonding information were collected by scanning electron microscope (SEM) and X-ray photoelectron spectroscopy (XPS). These results have important implications for the next generation of particle accelerators.

Abstract ID: 397

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Sandwich materials/hybrids, Multifunctional composite, Advanced composites

Keywords: Magnesium, Hybrid-metal matrix composite, Friction and wear, Wear mechanism.

In-situ ceramic reinforcement to develop Mg-based MMC and its tribological response

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Owing to its specific mechanical properties, Magnesium based alloys and composites are promising futuristic materials for structural, automotive and biomedical applications. Structure (clamping, riveting and bolting), piston cylinder, valves etc. are few areas where Mg-based components require to be wear-resistant.The present study explores the development of CeO2 and MgO particles through an in-situ reaction in the Mg melt. The developed MMCs are named as novel hybrid-metal matrix composite (h-MMC). The formation of CeO2 and MgO particles is confirmed using X-ray diffraction (XRD), Scanning electron microscope (SEM) and Energy dispersion spectroscopy (EDS). The compressive analysis of the developed h-MMCs showed improvement in strength and ductility both, which is unique observation. Wear and frictional responses have been recorded using Tribometer under pin-on-disk configuration for a range of speed and load under starved lubricated condition. The worn surfaces have been analyzed using SEM and EDS to comment on involvement of wear mechanism(s).

Abstract ID: 398

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Narrow Bandgap Materials and Devices

Keywords: Nanoscaled device, Lateral BJT, Charge Plasma

Nanoscaled Charge Plasma based lateral Bipolar Junction Transistors: A study

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The rapid growth and development in the communication sector around the globe has motivated the device researchers to design and develop small high performance portable devices. The development of mixed signal systems, such as, system-on-chip (SoC), where both analog and digital circuits are present on a single substrate is receiving a considerable attention by the researchers. The SoC can be efficiently realized by BiCMOS technology, as BiCMOS on silicon on insulator (SOI) is the only technology providing both domains together, bipolar for the best realization of analog part and the MOS for the realization of digital part. However, the realization of BiCMOS is difficult and expensive, as the integration of vertical BJT with the lateral MOSFET results in severe compatibility issues. These problems in realizing the BiCMOS for SoC have been addressed by replacing the vertical BJT with a lateral bipolar junction transistor (LBJT) on SOI. The LBJT on SOI results in low power consumption, high speed due to reduced parasitic capacitances, better isolation and large packing density. Further, in a thin film SOI-CMOS technology, vertical BJTs do not exist. Another important advantage of LBJT on SOI is that they are ideally suited to thin films and share the fabrication scheme of MOS devices without the performance degradation. Unfortunately on the flip side, the LBJTs on SOI suffers from the poor gain and cutoff frequency issues due to base width and base series resistance and low breakdown voltage. Further, the high temperature ion implantation processes to create emitter and base regions of BJT are also issues at nanoscale. Besides, the doping fluctuations and doping activations are severe at nanoscale and need to be addressed urgently. The focus of this work is to design, develop and the study of lateral BJT on SOI with improved performance. The concept of charge plasma will be used, wherein, the emitter, base and collector regions are not being realized by the conventional doping or ion implantation technique, however, by using metals of different work functions. Therefore, the charge plasma devices are free from the doping and high temperature fabrication related issues. In this work, charge plasma based lateral BJTs on SOI, partial SOI will be presented and will be compared with the conventional LBJT on SOI. The performance enhancement by charge plasma concept in terms of gain and cutoff frequency will be observed.

Abstract ID: 399

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Ferrites and Garnets

Keywords: Intrinsic-disorder, glassy magnetic behavior, Griffith's like phase

Study of Intrinsic-Disorder induced Glassy Magnetic behavior and Griffith's like Phase in Polycrystalline GaFeO3 Compound

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Polycrystalline GaFeO3 compounds have been prepared in single-phase by well-known solid-state reaction method at three different cooling rates during the annealing process and the detail magnetic properties have been studied from low temperature to above room temperature. Detail structural characterization of the three compounds is done using full Rietveld refinement of powdered XRD data. A higher mixing ratio of the Ga3+ and Fe3+ cations in their crystallographic sites is observed with a higher cooling rate during the sample preparation. Inverse magnetic susceptibility obtained at different applied magnetic fields and magnetic isotherms obtained at different temperatures around the transition temperature shows the development magnetic Griffith's like phase and existence of short-range magnetic ordering up to a temperature far above transition temperature in the compounds with higher cation mixing ratio. In these compounds, also a glassy magnetic behavior is observed below spin blocking temperature. Later behavior is studied by measuring the magnetic memory effect in temperature-dependent magnetization curves. Mixing of the cations develops the intrinsic-disorder in the system which is attributed as the origin for the development of glassy magnetic behavior and Griffith's like phase in the system.

Abstract ID: 400

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Industrial applications of composite materials

Keywords: MCM-41, MCM-48, MEA, BZA, AEEA, CO2-adsorption

Amine-functionalised Mobile Composite Matter for CO2 Capture

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Carbon capture using amine impregnated solid mesoporous composite adsorbents is a promising strategy due to convenient operation, low regeneration cost, outstanding cycle efficiency, and economical viability. In this work, as synthesized siliceous Mobil Composite Materials MCM-41 and MCM-48 are wet impregnated with Benzylamine as primary cyclic amine, Monoethanolamine as primary linear amine and Amino-ethyl-ethanolamine as secondary diamine to enhance CO2 adsorption capacity. The optimum amine loading, amine type, CO2 partial pressure and temperature on CO2 adsorption are investigated. The materials are characterized using N2-adsorption/desorption, XRD, TGA, FT-IR, FESEM and elemental (CHNS) analysis. The CO2 adsorption performances of MCM-41, MCM-48 and amine impregnated adsorbents are studied using isob-HP2 automated high pressure sorption analyzer instrument up to 30 bar of CO2 partial pressure and in the temperature range of 25-80°C. In the CO2 partial pressure range of 1 bar, the MCM-41-40%AEEA and MCM-48-30%AEEA materials are exhibited the CO2 adsorption capacity of 2.34 mmol/g and 3.33 mmol/g which are 3.5 times and 5.2 times higher than that of in MCM-41 (0.68mmol/g) and MCM-48 (0.637mmol/g) respectively. The materials are presented good structural and thermal stability. The adsorption capacity is decreases with increase in temperature due to exothermic property of CO2 adsorption. The Sips and Toth isotherm models are better suited to correlate experimental CO2 adsorption data in comparison with the Freundlich and Langmuir models. The isosteric heat of adsorption (ΔHiso) is calculated from Van't Hoff plot using iSorbHP-win software to understand the degree of heterogeneity and the surface energy distribution of the adsorbents. The CO2 adsorption capacity up to CO2 partial pressure of 30 bar and amine efficiency of MCM-48-30%AEEA are highest among the amine functionalized Mobil Composite materials reported in open literature. The MCM-48-30%AEEA is proposed as a promising adsorbent in low to high pressure post-combustion flue gas and natural gas purifications.

Abstract ID: 401
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Bio-composites
Keywords: avian eggshell, PBAT, PLA, electron-beam, gamma-radiation

STUDY OF EFFICIENCY OF IONIZING RADIATION IN PBAT/PLA BLEND REINFORCED WITH BIO-EGGSHELL

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Plastics global annual production exceeds 300 million tons and 99 % of the total plastic production is originated from oil or other fossil combustibles. When discarded, plastics oil based can last by centuries, posing a great threat for society and when burned, they release carbon dioxide in atmosphere, contributing for a global climate change. As an alternative, they are being slowly replaced by bioplastics, as PLA (poly-lactic acid) and PBAT (butylene adipate co-terephthalate). Food and dairy industries produce annually huge amounts of avian eggshells residues and their disposition constitute a serious environmental risk. Bio-load from avian eggshells as polymers reinforcement are based in their higher benefits as resistance and rigidity besides being a friendly environmental material, degradable and renewable. PLA and PBAT are thermoplastics capable to be processed by conventional methods: nevertheless, due to their high interfacial tension, it is required the use of compatibilizers. In this work, additives and heat generally used as compatibilizers were replaced by ionizing radiation: electron beam and gamma radiation, at 200 kGy dose. It was used PBAT/PLA 50/50, with avian bio-eggshell (bio-$CaCO_3$), 125 µm particle size, along with compatibilizers. Characterizations included: DSC, TGA, FTIR, XRD and mechanical essays.

Keywords: avian eggshell, PBAT, PLA, electron-beam, gamma-radiation.

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Abstract ID: 402

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Bio-composites

Keywords: Semiconductor Quantum dot, Diluted Magnetic Semiconductor, Human Serum Albumin, Biocomplex, 143 Osteosarcoma cells

Interactions of human serum albumin with II-VI semiconductor quantum dots with magnetic impurities probed by optical spectroscopy methods

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Semiconductor nanostructures have attracted great interest in different branches of science and technology. From point of view of biomedical applications II-VI semiconductor based quantum dots (SQDs) are the most studied. In addition, II-VI semiconductor compounds have another functionality as a basic matrix for diluted magnetic semiconductors (DMSs) [1]. Due to unique size dependent optical properties, SQDs can be successfully used as a novel probes in biosensors as well as bioimaging and biolabeling [2,3]. For such kind of applications, the interactions of SQDs with model proteins type of human serum albumin (HSA) play important role. In this work, we report of studies of interactions between II-VI based SQDs wit Mn and Co impurities and model proteins type of HSA. To probe this interaction, in addition to conventional UV-Vis absorption and photoluminescence spectroscopic methods we have used micro-Raman and FTIR spectroscopy. It was proved that, in all cases, the fluorescence quenching of HSA by the SQDs depends on the size and temperature. In the steady-state fluorescence studies, the interaction parameters including binding constants, number of binding sites, quenching constants were determined. Obtained data enable us to find optimal SQDs concentration useful for carcinoma cells bioimaging. However, in case of CdMnS-HSA biocomplex using for labeling this molecule, the concentration of SQDs should be higher than in CdCoS-HSA biocomplexes. The low toxicity as well as high stability of the SQDs - HSA biocomplex in the case of their using as bio-imaging probes for the 143b osteosarcoma cells has been demonstrated.

Key Words: Semiconductor Quantum dot, Diluted Magnetic Semiconductor, CdMnS, CdCoS, Human Serum Albumin, Biocomplex, 143 Osteosarcoma cells

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Abstract ID: 403

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster/Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices
Keywords: CsPbX3 perovskite, DFT, structural properties, electronic properties, optical properties

Electronic Structure and Optical Properties of Cubic and Orthorhombic CsPbX3 (X = Cl, Br, I) Perovskite: A Theoretical Understanding from DFT Calculations

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Caesium lead halides (CsPbX3) perovskite has recently attracted significant attention owing to its rapidly increasing competence when used for solar cells or light-emitting diode devices. In this study, we make a comprehensive density functional theory (DFT) calculation to determine the structural, electronic, and optical properties of cubic and orthorhombic temperature-dependent phases of CsPbX3 perovskite using the full potential linear augmented plane wave (FP-LAPW) method within the framework of the DFT, as implemented in the WIEN2k code. For this purpose, different exchange potentials: local density approximation (LDA), Perdew–Burke–Ernzerhof generalized gradient approximation (PBE-GGA), Engel–Vosko generalized gradient approximation (EV-GGA), Perdew–Burke–Ernzerhof revised for solids (PBEsol), modified Becke–Johnson generalized gradient approximation (mBJ-GGA), new modified Becke–Johnson generalized gradient approximation (nmBJ-GGA), and unmodified Becke–Johnson generalized gradient approximation (umBJ-GGA) were used. Our results on band structure indicate that the cubic and orthorhombic phases have direct energy bandgaps. Despite the large variations in their lattice constants, the two phases of CsPbX3 possessed almost similar optical properties. This result indicates a wide temperature range of operation for CsPbX3.

Abstract ID: 404

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Bio and Chemical Magnetism and Magnetic Fluids

Keywords: Microfluidic chip, Microchannel modeling, Study of fluid flow

Analysis of microfluidic design of 3D chip

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The highly integrated microfluidic chip can be used for multi sample operation, including many reaction steps. The speed of immune response on microfluidic chip can be improved due to the reduction of size. By controlling the flow of fluid in the micro-channel, the microfluidic chip can complete the separation and analysis of liquid samples.

In order to detect a substance by microfluidic immunoassay chip, it is necessary to simulate the fluid flow in microfluidic chip. Fluent is used to simulate the designed microfluidic chip and a better scheme is determined. When analyzing the flow situation and the flow field distribution of the liquid in the chip, we need to make a reasonable abstraction of the external environment and the system itself provided by the real world, and simplify some unnecessary conditions or conditions that have little impact on the system.

In this paper, the driving condition of microfluidics is equivalent to the velocity boundary condition at the entrance, i.e. a constant velocity is selected as the boundary condition at the entrance. We can select the calculation domain to be solved as a relatively independent part of the system, and directly use the three-dimensional model of all the research objects for calculation. We build a three-dimensional model of the flow part of the microfluidic chip. After we have determined the geometric region to be calculated, we need to discretize the geometric region, that is to say, we need to mesh it (unstructured grid and adaptive grid, etc.) as mentioned above. The model after solid grid division of microfluidic chip is shown. Fig. 3 is the vector space diagram of sample fluid velocity in the chip channel using the circular reaction pool. It can be seen from the diagram that the sample fluid to be tested has an acceleration process after entering the channel, and the velocity slows down after reaching the reaction area. The speed is evenly distributed in the circular space, which is conducive to the reaction charge for effective detection.

Abstract ID: 405

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster/Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Inkjet Printing, Flexible Electronics, Multilayer thin-film fabrication.

Monolithic Inkjet Printed Multilayer Thin-film Flexible Electronics Fabrication of Conductive, Resistive, and Dielectric Polymers

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Inkjet printing (IJP), a new additive fabrication process, makes it possible to produce lower-cost large area electronics in contrast to traditional microfabrication. IJP does so by depositing thin-film layers of various inks including conductive, semi-conductive, resistive, and dielectric materials on planar substrates such as glass or polymers [1]. We have been exploring various inkjet printing approaches as the sole monolithic IJP fabrication process for preparing thin-film low-cost flexible electronics with applications to wearables, Internet-of-things, and environmental monitoring. A Dimatix Material Deposition Printer (DMP-2831, Fujifilm, Dimatix Inc., NH) was used to print these inks on glass and other flexible substrates such as polyamide (PI). The printer cartridge (10 pL droplet size) has 16-inline MEMS-based nozzles with a 20µm pitch. Silver nanoparticle inks (Metalon JS-B40G from Novacentrix, Austin, TX, with 40% loading and average particle size of 60-80 nm) were printed as the conductive layer, with a 1.8 µm thickness and a 25 mΩ/square surface resistivity on PI [2]. Polypyrrole (PPy) (Sigma Aldrich, St Louis, MO) was tested for the resistive layer. Poly(4-vinylphenol) (PVP) and CuO inks were explored as dielectric layers, with PVP outperforming with respect to superior surface smoothness and lesser micropores observed and measured by SEM and AFM. Various compositions of Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) inks were tested with limited success. The best performing composition was 4 parts of 1.1% PEDOT:PSS solution with 1 part ethylene glycol (EG) that were annealed at 180˚C for 20 minutes. The contact angles on Si, PI, PVP, and Ag were 20.9˚, 55.7˚, 69.2˚, and 20.5˚, respectively, with a water contact angle on PEDOT:PSS of 19.73˚. The monolithic multilayer fabrication process was successfully utilized to develop metal-insulator-metal capacitors, multilayer resistors, and flexible printed circuit boards.

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Abstract ID: 406

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Lithium Ion Batteries

Keywords: Energy storage, Lithium-sulfur batteries, Porous carbon materials

Biomass-derived porous carbon materials for high energy lithium-sulfur batteries

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Among many types of energy storage technologies, lithium-sulfur batteries (Li-S) are becoming a promising option, which would actually overcome limitations of Li-ion technology. In contrast to Li-ion batteries, which usually utilize graphite and transition-metal oxides, Li−S cell consists of a metallic lithium anode and a sulfur composite cathode. Metallic lithium is characterized by a very high electronegativity and low density, means it provides a high theoretical specific capacity of 3861 mAh g-1. Sulfur, one of the most abundant elements in earth's crust, possess a high theoretical capacity of 1673 mAh g-1 and it is considered to be safer battery component compared to Li-ion battery chemistries. Sulfur cathode coupled with lithium-metal anode can deliver high theoretical gravimetric and volumetric energy densities of 2500 Wh kg−1 and 2800 Wh L−1, respectively.

Apart from the theoretical potential, Li-S system still suffers diverse challenges. Lithium polysulfides shuttle is one of those aspects as it results in low charge efficiency, fast capacity loss as well as severe anode corrosion. For this reason the suppression of the redox shuttle mechanism is a high priority task.

Incorporating active sulfur into carbon frameworks with good electrical conductivity and diverse nanostructures, such as micro/mesoporous carbons, have been regarded as one of the most effective strategies to enhance the electrochemical performance of lithium sulfur batteries.

In our research high surface area, biomass-derived carbon materials have been prepared by means of chemical activation of waste organic materials with potassium carbonate and investigated as novel sulfur cathode component for lithium-sulfur batteries. As evidenced by scanning electron microscopy and nitrogen absorption isotherms, the synthesized material features hierarchical micro-macroporous structure with sponge-like arrangement of interconnected microfilaments. Composite carbon/sulfur cathode exhibits large initial specific discharge capacity of 886 mAh g-1, which remained remarkably stable over subsequent 50 charge/discharge cycles (capacity loss less than 1%). Excellent reversibility and cyclic stability of this composite cathode has been attributed to a unique combination of micro and macroporosity, allowing for the retention of the intermediate polysulfides within the carbon framework, without excessive dissolution in the bulk of electrolyte.

Key Words: Energy storage, Lithium-sulfur batteries, Porous carbon materials

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Abstract ID: 407

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Nanostructured materials for advanced batteries

Keywords: Lithium-sulfur batteries, Lithium polysulfides, Permselective membranes

Efficient suppression of lithium polysulfides by permselective membranes for lithium-sulfur batteries

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The unique properties such as high theoretical capacity, energy density, low cost and environmental benignity have identified lithium-sulfur batteries as a potential successor of lithium-ion batteries. Although, low conductivity of elemental sulfur, shuttling of polysulfide between cathode and anode and undesirable high reactivity of metallic lithium impede this system from practical application. Numerous strategies have been undertaken to mitigate abovementioned limitations for e.g. various porous carbon materials have been adopted to enhance electronic conductivity and hinder the dissolution of lithium polysulfides into the electrolyte.

In the present work, hybrid nanoparticle consisting of BaTiO3 chemically coupled to graphene oxide (GO) sheets was synthesized and coated on either side of commercially available Celgard 2320 separator along with biomass derived activated carbon obtained from sisal fibres. This tri-layer permselective membrane with BaTiO3/AC, graphene oxide/AC and BaTiO3-g-GO/AC employed to Li-S cell delivered an initial discharge capacities of 1450, 1150 and 1000 mAh g-1 at 0.1C-rate respectively. The permselective membrane coated with BaTiO3-g-GO/AC has extraordinarily suppressed the self-discharge of Li-S with 90% of its total capacity even after 240 h which opens up the venue for lithium-sulfur batteries to achieve long cycle life without self-discharge for the applications in electric vehicles.

Key Words: Lithium-sulfur batteries, Lithium polysulfides, Permselective membranes

Acknowledgment:

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Abstract ID: 408
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Porous and cellular materials
Keywords: porous bioceramics, alumina, pore model, image processing

Three-dimensional model in assessing the pore geometry of a biomaterial intended for implantation

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Porous biomaterials are widely used in medicine. The right size of pores and connections between them decide about tissue penetration and mineralization, providing a good and durable connection of the implant with the bone. In addition, porous biomaterials are ideal drug carriers because they allow for the placement of a drug substance in the open pores of a biomaterial, and then its introduction directly into the human body during implantation. However, materials with porous structure have to meet strict requirements regarding open and total porosity as well as the size and shape of pores. Various research methods are used to characterize the pore geometry of biomaterials. Most of them are invasive or only allow for the analysis of pores present on the material surface. An alternative to characterizing the geometric structure of material pores is the use of computer modelling and simulation.

The main objective of the study was to develop a three-dimensional model of ceramic biomaterial pores, which would enable to determine the geometric parameters of pores, including their volume. The model creation process consisted of three main stages. The first one involved setting up the assumptions that the model should meet. As part of this stage, measurements were performed using a LEXT OLS4000 confocal scanning laser microscope. The research material consisted of samples of a porous corundum biomaterial produced by chemical foaming. The acquired images were analysed using the Image Metrology SPIP software, which allowed for the separation of pores from the surface image and their measurement. Based on the obtained parameters, the model assumptions were adopted. The next stage was implementation. The model was implemented in the Matlab environment. In order to allow the user to enter the input parameters of the model, a graphical user interface was designed and implemented. The user has the option of specifying the size of the model, the number of pores and the minimum and maximum pore diameter. Based on these parameters, a three-dimensional model is generated. Another element is the possibility of choosing the plane and the position of the cross-section. Based on the model, a computer simulation was carried out, resulting in a three-dimensional representation of the biomaterial pores and its cross-section. By generating the cross-section, the user obtains a flat image of the surface showing the pores located in a given position of the cross-section and in a given plane, as well as the parameters characterizing the biomaterial pores.

Abstract ID: 409

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Dielectric materials

Keywords: high-k, gate dielectric, plasma-enhanced atomic layer deposition, Ga2O3, MOS capacitor

Investigation of Ultrawide Bandgap Ga2O3 MOS Capacitors with High-k Gate Dielectrics by Plasma-Enhanced Atomic Layer Deposition

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Today's power electronic systems for power generation, conversion, transmission, etc. demand very high power of mega- to giga-Watt (which requires high voltage of 1~100 kV and high current of 1~100 kA) and high energy efficiency (which requires high energy conversion rate). One of the key components in power systems are power electronic devices such as transistors, diodes, thyristors, etc. which provide the core functionality of power electronic systems. Conventional Si devices are limited to operation at low junction temperatures and low voltages by the materials properties of Si. The emerging single-crystal beta-gallium oxide (β-Ga2O3) is more desirable due to its unique ultra-wide bandgap energy (Eg=4.8 eV) and high breakdown strength (EC=8 MV/cm), which result in the superior Baliga's figure of merits. In this paper, we study the chemical, structural, and electrical properties of Ga2O3 metal-oxide-semiconductor (MOS) capacitor with high-k hafnium dioxide (HfO2), zirconium dioxide (ZrO2) and their stacks as gate dielectric. High-k dielectric provides a physically thicker film with equivalent capacitance, therefore better exploits the high breakdown strength of Ga2O3 in its MOSFET devices. The high-k films were deposited using plasma-enhanced atomic layer deposition (PEALD), and post deposition annealing was performed at different temperature and ambient. The atomic structures, interface state densities and dielectric strength of the high-k films were characterized and the optimized film parameters and process were derived.

Abstract ID: 410
Symposium 4: Functional Composite Materials (FCM)
Poster/Oral Presentation
Topics: Nanocomposites
Keywords: Ultrafast self-assembly, MoS2/Cu(OH)2 nanowires, Humidity detection, Self-recovery ability, highly sensitive

Ultrafast self-assembly MoS2/Cu(OH)2 nanowires for highly sensitive gamut humidity detection with enhanced self-recovery ability

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Humidity sensors have attracted intense interests in various fields due to the importance of humidity detection. Different methods have been adopted to enhance sensing performances of humidity sensors, while it is challenging for researchers to avoid the invalidation of the sensors after being wet. Here, we for the first time introduce self-assembly MoS2/Cu(OH)2 nanowires fabricated by liquid self-spreading-coating-evaporating as sensing materials and present MoS2/Cu(OH)2 nanowires based quartz crystal microbalance gamut humidity sensors with superior sensitivity and self-recovery ability. The sensors deliver a remarkable sensitivity (60.8 Hz/%RH) under a wide range (0 – 97 %RH) with fast response (1.9 s)/recovery time (3.8 s) and upgrade self-recovery ability that can maintain their original performances even after being wet, frozen and heated or immersed in water. The sensors are also employed to monitor water counting, dew alarming, and human breathing (within 4 s), further showing their ultrahigh sensitivity for water molecules. The underlying humidity sensing mechanism is interpreted by DFT calculations and in-situ FTIR experiments adequately, revealing that the high sensing performances are attributed to abundant adsorption sites and physisorption of water molecules. Our work proposes a strategy for transferring materials to arbitrary nanostructures swiftly and demonstrates new perspectives for highly sensitive humidity detection as well as self-recovery ability.

Abstract ID: 411

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: All solid-state batteries

Keywords: aluminium ion, battery, red phosphorous, porous carbon, biomass.

High capacity and high voltage cathode material for rechargeable aluminium ion battery

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Development of high specific capacity cathode operating at higher voltage can lead to the development of rechargeable aluminium ion battery as a promising energy storage device for large scale application. Herein a cathode structure is designed with red phosphorous nanoparticles embedded in disordered carbon nanosheets (Red P@DCNS) from a cost effective resource (Betel nut fruit shell) by a simple and scalable technique. The combined interaction of red phosphorous and DCNS with aluminium ions enables to achieve a specific capacity of 350 mAh g-1 at 30 mA g-1 with a high operating voltage of 1.95 V. Moreover, the smaller size and strong chemical bonding of red phosphorous to DCNS facilitates for the stable capacity over 500 cycles with a coulombic efficiency of nearly 100 %. Red P@DCNS possess both high discharge voltage of 1.95 V and higher specific capacity surpassing the aluminium ion batteries previously reported. It is also evident that reversible formation of aluminium phosphate is responsible for the higher specific capacity of the battery. These findings are of great significant and provide a new concept of designing a high voltage cathode and can lead to further advancement towards the development of rechargeable aluminium ion battery.

Abstract ID: 412
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Fiber reinforced Composites
Keywords: Concrete, Radiation, Gamma ray

Gamma Attenuation Properties of Special Concrete

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The rapid development in science technology makes nuclear technology widely used in electricity generation, industry and medical care, which have increased people's contact with different kinds of radiation. Three main methods for protection from radiation are usually utilized; these are time, distance and shielding. Among the three methods, shielding is the most important in which shielding materials become important. Radiation shielding is of significant importance due to the fact that nuclear technology is widely used in different fields such as industry, medicine, agriculture, and scientific research. Since different types of radiation (X- and gamma rays, alpha particles, beta particles, and neutrons) interact in different ways with shielding material, the type and energy of the radiation must be taken into account in order to increase the effectiveness of shielding materials. Among the various types of radiation, gamma radiation has one of the highest material penetration capabilities. Therefore, gamma radiation shielding capability of construction materials needs to be developed in order to improve the radiation protection of humans and the environment. The attenuation characteristics of shielding materials are related to the atomic mass number, density, thicknesses, photon absorption cross sections, and incident photons' energy. Concrete is the most commonly used shielding material due to the fact that it is cheaper, easier to mould into complex shapes, and suitable for neutron and proton shielding. The main purpose of the radiation shielding concrete design is to provide shielding against gamma, X-rays and the neutrons that have strong penetration ability. Gamma and X-rays can be absorbed by aggregates containing heavyweight elements, such as barite, magnetite, hematite, etc., with high density. Such properties have been extensively used in the previous studies to reduce above-mentioned photons' impact .Moreover, moderate and slow neutrons can be absorbed by only low-atomic weight elements such as hydrogen, boron, carbon, etc. Therefore, a properly designed radiation shielding concrete should also include both light and heavy-atomic weight elements together.

Radiation-shielding properties of three concretes prepared using different precursors such as ferrous waste with other mineral additives such as ground granulated blast furnace slag and fly ash were investigated comparatively with ordinary concrete mixture. In addition, the mechanical performance of all specimens was evaluated in terms of their flexural and compressive strength.

Abstract ID: 413

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multiscale Modeling in Mechanics and Composite Materials

Keywords: Peridynamics, Fracture, Nanoscale phase separation

Fracture Mechanics of Phase-Separated Glasses by Peridynamics Simulations

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Although oxide glasses have many unique properties, their range of applications remains limited by their brittleness. By mimicking the microstructure of composite materials, the presence of controlled nanoscale phase separation in glass could overcome this limitation. However, the nature of the toughening mechanism induced by such nanostructuring remains poorly understood. Here, based on peridynamic simulations, we investigate the effect of nanoscale phase separation on the crack propagation mechanism. We show that phase separation can significantly increase glass's toughness (with up to a 90% increase in the fracture energy for the range of conditions investigated herein). The extent of toughening is found to arise from a balance between the overall cohesion of the phase-separated glass and the propensity for crack deflection. This suggests that controlled nanoscale phase separation is a promising route toward the development of tough, yet optically transparent glasses.

Abstract ID: 414
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Nanocomposites
Keywords: epoxy, nanoclay, high shear, interface, viscoelasticity

Effect of surface treatment on viscoelastic behavior of epoxy nanocomposites

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Properties of most polymeric composites depend on processing parameters including curing temperature and time to a great extent leading to formation of network of polymer chains. However, in reinforced polymer composites, properties are mostly dictated by the interfacial chemistry and subsequent interaction between filler materials and polymers molecules along with the aforementioned factors. viscosity and subsequent heat of reaction and activation energy of reaction were significantly affected. cure Surface modifications of montmorillonite nanoclay also affected gelation time leading to different cure time at various temperatures.

Nano-composites of epoxy clay have been studied where epoxy is mixed at high shear rates with clay . In our method of making nano-composites, an epoxy, Diglycidyl ether of bisphenol (DGEBA) A was mixed under high shear with organically modified mica type silicate (OMTS) either of Benzyl Dimethyl Stearyl Ammonium (BDSMA), Cloisite 10A or of methyl Bis hydroxyethyl Methyl Stearyl Ammonium chloride(BMSA), Cloisite 30A ion exchange with sodium montmorillonite. Dynamic viscoelastic deformation was analyzed to determine Equilibrium Plateau Modulus that showed power law dependence on filler and temperature. Flexible chain filler, Cloisite 30A in the epoxy shows less temperature dependence than Cloisite 10A in the epoxy at the same filler concentration.

Abstract ID: 415

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Contacts to Semiconductor Epilayers, Nanostructures and Organic Films

Keywords: photoreceptor, image, polymer film, filler, wear

A model of photoreceptors brittleness and wear

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Photoreceptor is a central device in digital printers. The top layer, Charge Transport Layer made up of polycarbonate and Charge Transport Molecule is susceptible to abrasion by stresses of developing system or cleaning system when it is repeatedly used in printing process. The abrasion of the photoreceptor causes deterioration of electrical properties such as lowering sensitivity or lower charging and results in irregular image such as lower image density and image stain. Single and multiple coating were made with filled and unfilled binder polymers and their modulus and hardness were measured by nano-indenter. Charge Transport Molecule reduced Tg, increased modulus and reduced strain to photoreceptor wear rate. Addition of nano-filler silica in the polymer either polycarbonate or polyester increased strain to break with increased photoreceptor life the resulting charge transport layer exhibits enhanced cracking suppression, improved wear resistance, excellent imaging member electrical performance, and improved copy print out quality.. Transfer members useful in electrostatographic reproducing apparatus, including digital, image-on-image and contact electrostatic printing apparatus. The transfer members feature a substrate comprising a nanosize polymer material and can be used as transfer members, transfuse, transfix members, or transport.A model based on interaction between nano-filler and polymer resulting in improved composite electronic material and its effect on image is proposed and verified.

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Abstract ID: 416
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Porous and cellular materials
Keywords: Nanoporous material, sorption isotherm, gas separation

De Novo Inverse Design of Nanoporous Structures by Machine Learning

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Nanoporous materials (e.g., zeolite, activated carbon, metal-organic framework, polymeric membranes, etc.) have various technological applications, including gas separation, gas storage, catalytic transformations, etc.1,2 The behavior of nanoporous materials (e.g., their sorption isotherm, that is, the amount of adsorbed gas as a function of partial pressure) strongly depends on their pore size and shape distribution. Importantly, the design of new nanoporous materials with tailored structures could enable new breakthroughs in our ability to separate CO2 from a given flue gas (a prerequisite to CO2 capture).3 However, our ability to discover new nanoporous materials with tailored functionalities has thus far been plagued by the virtually limitless degrees of freedom involved (i.e., infinite number of potential nanostructures). Here, we present an innovative framework combining high-throughput simulations and machine learning to accelerate the inverse design of nanoporous phases featuring a targeted sorption isotherm.4 Our approach consists in (i) hard-coding a lattice-based density functional theory gas sorption simulation as a convolutional network (CNN) in TensorFlow to leverage the automatic differentiation functionalities of TensorFlow (as differentiability simplifies our inverse design problem) and (ii) using this CNN model to efficiently train a deconvolutional network that generates optimal nanoporous structures. This approach enables the de novo design of non-intuitive nanoporous structures featuring unusual sorption isotherms.

Abstract ID: 417

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: Oxygen; Graphene oxide; Single walled nanohorn; Fluorinated poly (ethylene glycol); OH terminated dendrimer, Pentafluoropropionic acid; Thermogravimetric analysis.

Single walled carbon nanohorns and graphene oxide sheet based oxygen delivery system.

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Oxygen has a vital role to maintain normal physiological function of human body. It has a crucial role in cellular microenvironment which controls cell viability, differentiation, Adenosine triphosphate (ATP) production, and regulating metabolic processes. In response to oxygen gas for therapy, we prepared oxygen conserving platforms of carbon nanohorns and graphene oxide (GO) and its composites. Fluorinated poly (ethylene glycol) (F-PEG) and fluorinated dendrimer (F-Den) were functionalized with single walled carbon nanohorn (SWCNH), graphene oxide (GO), and nitrogen doped SWCNH (N-SWCNH), to prepare the composites of F-PEG@SWCNH, F-PEG@GO, F-PEG@N-SWCNH, F-Den@N-SWCNH and F-PEG@F-Den@N-SWCNH as an effective oxygen delivery system. Characterization of the composites were done by TEM, Fourier transform infrared absorption (FTIR) spectra, Raman scattering spectra, thermogravimetric analysis, X-ray diffraction (XRD) and XPS. The maximum oxygen conservation of SWCNH, F-PEG@SWCNH, GO and F-PEG@GO at 24 h was measured. Moreover, the oxygen uptake capacity of N-SWCNH, F-PEG@N-SWCNH, F-Den@N-SWCNH and F-PEG@F-Den@N-SWCNH was observed during 48h. The existence of F-PEG and dendrimer in the composite, F-PEG@SWCNH, F-PEG@GO, F-PEG@N-SWCNH, F-Den@N-SWCNH and F-PEG@F-Den@N-SWCNH cause to intensify the oxygen uptake efficiency. The prepared formulations might be potential used for oxygen gas delivery system showing the ability to store and release gas slowly over time.

Abstract ID: 418
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Porous and cellular materials
Keywords: Disordered Materials, Stiffness, Molecular Dynamics, Machine Learning

De Novo Prediction of Light yet Stiff Disordered Atomic Structures by Machine Learning

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The evolution of the Young's modulus (E) of disordered materials (e.g., glasses) as a function of their density (ρ) is typically governed by some scaling laws E ~ ρ^n, wherein less efficiently packed structures (i.e., lower ρ) are also less stiff (lower E). The drop in stiffness upon decreasing density is governed by the scaling exponent n, wherein larger scaling exponent results in a more pronounced drop in stiffness. Here, by combining high-throughput molecular dynamics (MD) simulations and Bayesian-optimization-based machine learning (ML), we predict the existence of a "stretching-dominated" family of disordered networks exhibiting minimum scaling exponent. This paves the way toward the design of new ultralight, yet ultrastiff non-crystalline phases.

Abstract ID: 419

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Porous and cellular materials

Keywords: Phase separation, Polydimethysiloxane, Porous cell culturable membrane

Thin porous PDMS membrane prepared by phase separation method and its applications for cell culture

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Cell culture inserts such as Transwell® insert with a porous membrane growth surface are useful in cell biology. Common cell culture membranes are made from polyethylene terephthalate (PET) or polycarbonate (PC), both of which are rigid polymers and not appropriate for cells that require a deformable membrane, such as lung and gut cells1-2. Moreover, the porosity of PET membranes are too low (< 1%) to study cell biology. While PC membranes have higher porosity (ca. 20%), cell observation is difficult due to its semi-transparency. In this study, we use a spin-casting assisted polymer blend phase separation method to prepare thin, porous, and flexible membranes for cell culture3-6. Specifically, polydimethylsiloxane (PDMS) and polystyrene (PS) were choose for the experiment7. PDMS is a low elastic material which can easily to perform the reversible deformation needed during observation. By selectively etching PS components into the blend membrane, a porous PDMS structure was fabricated on the membrane. Furthermore, we can adjust the thickness of the membrane, and the connectivity of PS domains by changing the concentration and blend ratio between PDMS and PS, which affects the pore size and the pore density on the final membrane. In summary, we prepared a deformable, thin, and porous PDMS membrane by a polymer blend phase separation method, which has a higher porosity compared to that of common cell culture inserts and cell culturable membranes.

Abstract ID: 420

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Synthesis, self-assembly, nanomaterials, gas sensing, combinatorial nanofabrication

Fabricating Three Dimensional Self-Aligning Nanoparticle-based Structures as Gas Sensor Array

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Three-dimensional (3D) nanoparticulate bridge structures are demonstrated as room temperature operated, low power gas sensors in this study. 3D morphologies have potential to overcome technological/economic challenges faced in 2D planar homogenous film applications. Fabricated using gas phase electrodeposition, this concept can guide charged nanoparticles to predetermined locations on a surface with sub micrometer resolution. Sequential shutter free deposition is possible, preventing use of additional steps for lift-off and improving material yield. The developed device - a room temperature operated sensor chip; can integrate an array of different nanostructured materials arranged in a pre-decided pattern on the substrate. Each gas sensitive structure is a 3D nanobridge, composed of porous but electrically conducting nanoparticle network. Method of gas phase electrodeposition has been reported [1] and used as interconnects in nanoelectronics. Extending the basic principles for self-aligned growth of nanobridges with a new substrate design, it is possible to grow bridges of different materials on a single substrate to accomplish a single chip “electronic nose” like sensor array with orthogonal sensing capabilities and multi gas sensitivity and selectivity. From an experimental point of view, the method uses a spark discharge-based nanoparticle source in combination with sequentially biased surface electrodes and charged photoresist (dielectric) patterns to accomplish electrodeposition. In total, 1080 Platinum, Nickel oxide and Gold nanobridges are grown to detect Ammonia, Carbon Monoxide and Hydrogen Sulfide gases, respectively. Response and recovery times for these sensors at three different target gas concentrations are reported. The as-deposited bridges have a sensor drift, which can be decreased by 80% with a stabilization cycle of exposure and removal of target gas. The final gas sensor can detect target gases within minutes and have low sensor signal drift. Additionally, this study highlights the challenges that need to be systematically studied to realize the full potential of programmable approach towards gas phase electrodeposition.

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Abstract ID: 421

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster/Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: Two-Dimensional Materials, Energy Storage, Ion-Battery, Density Functional Theory, Molecular Dynamics.

Computational Modeling of Two-Dimensional Materials for Sustainable Energy Storage

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Two-dimensional materials (2DM) such as graphene, transition metal dichalcogenides (TMD), MXenes, and their heterostructures are among the most promising energy materials for the radically advanced batteries. In this talk, two important computational aspects of 2DM-based batteries are addressed – (i) 2DM as anode materials, and (ii) 2DM as van der Waals (vdW) slippery interface. The conventional anode materials have several problems, such as low gravimetric capacity (e.g., graphite – 372 mAh/g) and high volume expansion (e.g., silicon – 300%). Our computational modeling shows that topologically modified 2DM can be utilized as high-capacity anode materials for ion batteries with capacity as high as 1000 mAh/g. However, despite enormous opportunities in 2DM anode, several challenges need to be addressed, such as trapping of adatoms at the defect sites, the effect of defects on the diffusivity of adatoms, mechanical degradation at defect sites during charging/discharging, etc. The second part of the talk discusses the interface of anode and current-collector (e.g., silicon anode and copper current-collector in Li-ion battery). To combat the issue of high-stress development at the anode-current collector interface during charging/discharging, we propose the usage of the graphene layer over the current collector as a vdW slippery interface that reduces the interfacial stress and enhances the cycle life of batteries. Our computational results are in excellent agreement with the experimental findings.

Abstract ID: 422
Symposium 4: Functional Composite Materials (FCM)
Poster/Oral Presentation
Topics: Synthesis and characterization of Composite materials
Keywords: Nanocomposite, Ionic liquid, Polymer gel, Double network

Development of silica nanoparticles/poly(ionic liquid)s composite double-network ion gels for gas separation membranes

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Ion gels are a new class of ionic liquid (IL)-based soft materials consisting of a three-dimensional polymer network and incorporated free IL. Recently, ion gels have attracted considerable interest for their applications in electrochemical devices, actuators, and gas-separation membranes [1]. However, low mechanical strength of ion gels is still an issue to overcome the limitation in practical applications. Here, we developed tough, thermally stable, and high water-resistant double-network (DN) ion gels consisting of a partially clustered silica nanoparticle network and poly(ionic liquid)s (PILs) network holding a large amount of free IL. Tensile stress measurement showed that the silica nanoparticles/PILs DN ion gel had more than four times higher fracture stress than the PILs single-network ion gel. We also found that the mechanical properties of the silica nanoparticles/PILs DN ion gel were enhanced as the diameter of silica nanoparticles decreased. In addition, cyclic tensile measurement of the silica nanoparticles/PILs DN ion gel showed hysteresis loops, suggesting that their enhanced mechanical properties are achieved by an energy dissipation mechanism analogous to the DN principle; the first partially clustered silica nanoparticle network is ruptured when a large strain is induced [2]. Thermal gravimetric analysis showed that the silica nanoparticles/PILs DN ion gel had a decomposition temperature around 400 °C, which was derived from the second cross-linked PILs network. Furthermore, swelling test clearly showed that the silica nanoparticles/PILs DN ion gel had an excellent water-resistant property derived from hydrophobic nature of the cross-linked PILs network. We believe that such PILs-based DN ion gels can be used as carbon dioxide separation membranes, sensors, and actuators for soft robotics.

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Abstract ID: 423

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Advances in electrolyte and electrolyte additives

Keywords: Lithium-sulfur batteries, Lithium polysulfides, UV-Vis spectroscopy

Electrochemical and transport phenomena in Li-S cells with novel electrolytes studied with UV-Vis

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Lithium-sulfur (Li-S) cells are widely considered as one of the most promising candidates for the next generation, high energy density energy storage devices. The need for a substantial breakthrough in battery energy densities becomes more and more obvious as electric vehicles and portable electronic devices become ever more widespread. In spite of a significant progress that has been made in the field of Li-S battery developments, a lot of works is still necessary to understand certain basic phenomena and mechanisms occurring during the operation of these power sources. Some of the most important unresolved issues in Li-S cells are related to the electrolytes and their interaction with carbonaceous cathode materials. In the present contribution it is intended to study how different new electrolyte compositions function in connection with mesoporous porous carbons. To elucidate the involved mechanisms, advanced UV-Vis techniques are applied with the ultimate goal of finding connections between the electrolyte compositions and kinetics of lithium polysulfide generation, transitions and transport within the electrochemical cell. The most promising combinations of carbons with new electrolytes are proposed and demonstrated in a Li-S cell.

Abstract ID: 424

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster/Oral Presentation

Topics: Theory of graphene, Mxenes and other two-dimensional materials

Keywords: Nanotechnology, 2D Structure Prediction, Self-Assembly of DNA bases, DNA biosensors

First-Principles Periodic 2D Structure Prediction of DNA Bases

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Deoxyribonucleic acid (DNA) contains the genetic information of all known living things and therefore it can be considered as the most important biomolecule in the world. The self-assembly of nucleic acid (NA) bases into well-organized hierarchical nanostructures has attracted much attention in recent years. The structures of DNA base molecules which show distinct patterning on two dimensional (2D) surfaces can potentially be used for applications of functional nanomaterials as biosensors. This motivation leads us to develop a new method; FFCASP (Fast & Flexible CrystAl Structure Predictor) for predicting 2D periodic structures of DNA bases. FFCASP generates the DNA base structures by global optimization of an intermolecular interaction potential that based on the symmetry-adapted perturbation theory combined with density functional theory (DFT-SAPT). In FFCASP, global optimizations have been carried out by a fully parallelized hybrid approach of particle swarm optimization (PSO) and simulated annealing (SA) algorithms. This methodology has been used to predict the 2D structures (such as filament, ring and network) of DNA bases. The results that are obtained so far have shown that besides the method is able to reproduce the known motifs which is captured by scanning tunneling microscopy (STM) images that contained in self-assembled structures of individual NA bases, it can also produce the new low-energy 2D surface structures. This study can provide insights into the self-assembly formation mechanism of DNA bases and thus it can open new horizons in different application areas such as organic electronics, organic photovoltaics and sensors in which predicting the 2D organic monolayer structures is essential.

Abstract ID: 425
Symposium 4: Functional Composite Materials (FCM)
Poster/Oral Presentation
Topics: Concrete and cementitious composites
Keywords: atomic structure, cement, calcium silicate hydrates, carbon footprint, molecular dynamics simulation

Decoding the Atomic Structure of Cement Hydrates

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Concrete is by far the most manufactured material in the world. However, the atomic structure of its calcium–silicate–hydrate (C–S–H) binding phase remains debated. This arises from the disordered, heterogeneous, multiscale nature of cement hydrates, which prevents the use of conventional experimental techniques to access its atomic structure. Here, we reveal the atomic structure of C–S–H based on force-enhanced atomic refinement (FEAR) simulations. Our atomic model offers an unprecedented description of the structure of C–S–H for varying compositions, both in terms of agreement with diffraction data and energetic stability. An accurate knowledge of the atomic structure of C–S–H is key to accelerate the nanoengineering of novel cementitious binders with enhanced properties or lower carbon footprint.

Abstract ID: 426

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Porous and cellular materials

Keywords: Capacitive deionization, tubular carbon electrodes, hierarchical porous structure, nitrogen/sulfur co-doping

Heteroatom N,S co-doped open hollow tubular porous carbon as electrodes for boosting capacitive deionization performance

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Heteroatom N,S co-doped open hollow tubular porous carbon (N,S-HTPC) materials were successfully fabricated via a facile MnO2-nanorod template method and utilized as electrodes for capacitive deionization (CDI) to achieve high-performance water desalination. In this research, carbon, nitrogen and sulfur sources were derived from LB agar coupled with β-cyclodextrin, which formed a hydrogel (LB agar@β-CD hydrogel) as precursor of N,S-HTPC. The as-prepared N,S-HTPC not only obtained excellent heteroatom co-doping properties but also owned a unique open hollow tubular structure with a hierarchical porous tube wall, a large specific surface area and abundant surface functional groups. As expected, the N,S-HTPC electrodes showed a high electrosorption capacity of 12.05 mg g-1 in 25 mg L-1 NaCl solution and an excellent cycling stability over 30 cycles. The excellent performance was mainly attributed to its open hollow tubular channels to decrease the internal resistance, hierarchical porous tube wall to transport and store ions, and the co-doped nitrogen and sulfur element in N,S-HTPC to achieve the higher conductivity and surface wettability. The high-performance and energy-efficient continuous deionization performance of N,S-HTPC made it to be a potential material for CDI technology.

Abstract ID: 427

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Solar Cells

Keywords: Defects, Perovskites, Electron-hole recombination, Electron-phonon coupling, Time-dependent density functional theory

Peculiar Defects Behavior in Charge Recombination of Metal Halide Perovskites and Conventional Semiconductors

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Metal halide perovskites have attracted great attention due to their high and rapidly rising power efficiencies, as well as many other important advantages. Since the low-cost solution-based synthesis of the perovskites invariably introduces defects, a strong defect tolerance should exist in these materials. However, it is usually believed that those defects would form Shockley-Read-Hall (SRH) electron-hole recombination centers that decrease solar conversion efficiency. Herein we investigate the non-radiative recombination processes in both MAPbI3 and CsPbI3 using ab initio non-adiabatic molecular dynamics within real-time time-dependent Kohn-Sham formalism and surface-hopping framework. Regardless of whether the defects introduce a shallow or deep state in the band structure, we find that the charge recombinations in these perovskites are not enhanced which contrary to predictions of the SRH theory. We show that the strong tolerance of electron-hole recombination against defects is explained due to the combination of having low-frequency lattice phonons and weakly overlapping electron and hole states. Both factors significantly decrease the non-adiabatic coupling and inelastic electron-phonon interactions. The previous SRH models that work for the conventional semiconductors, fails for the metal halide perovskites because they do not explicitly include the electron-phonon coupling. Thus, we propose that other “soft” semiconductors, in particular, a small bulk modulus should exhibit defects properties similar to those of the perovskites.

Abstract ID: 428
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Concrete and cementitious composites
Keywords: Nano technology, Nanosilica, slump flow, J-ring, V-funnel, L- box and U–box, Mechanical properties

COMPARATIVE ANALYSIS OF SELF COMPACTING CONCRETE USING NANO-TECHNOLOGY

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Nano-technology is a standout amongst the most dynamic research regions which has wide applications in practically every one of the fields. As concrete is most usable material in development industry it's been required to improve it's quality. Improving solid properties by expansion of nano particles have demonstrated noteworthy improvement than traditional cement. Essentially, nano-technology improves the material's mass properties and furthermore control or control materials at the nuclear scale to get more slender last items and quicker setting time. The extraordinary chemical and physical properties of nanomaterials empower a few applications extending from basic reinforcement to environmental pollution remediation and generation of self-cleaning materials. It is realized that solid is the main material in auxiliary applications, where firmness, quality and cost assume a key job in the high strength properties of concrete. This paper depicts the era to find the effect of nanosilica on self compacting concrete with fresh properties of concrete using slump flow, J-ring, V-funnel, L- box and U–box & effect on mechanical properties of self-compacting concrete using nanosilica.

Abstract ID: 429

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Polymeric composites

Keywords: Positive biopolymer, Photosensitivity, Gold nanoparticle, Volume Alteration

Positive Photoresponsivity of β-Cyclodextrin Modified Biopolymeric Composite

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Positive photoresponsive hydrogel offers volumetric expansion with the increasing photo intensity which is the reverse phenomenon of the negative photoresponsive hydrogel. Poly (N-isopropylacrylamide) is used as negative hydrogel [1]. The copolymer of polyacrylamide (PAAm) and acrylonitrile (AN) (PAAm-co-AN) [2] and the interpenetrating network of PAAm with polyacrylic acid (PAAc) i.e. PAAc-co-PAAm [3] are the widely used positive hydrogel by the association and dissociation of hydrogen bonding between PAAc-PAAm molecules under photo irrediation. The reported works on PAAc-co-PAAm was synthetic in nature and there was no report on their biocompatibility. In contrast, this work has modified the synthetic PAAc-co-PAAm with β-Cyclodextrin (β-CD) to make the polymer biocompatible. Another point of using β-CD is to improve the solvent encapsulation than the reported synthetic PAAc-co-PAAm. The existing research was showed irreversible stimuli dependent swelling where as in this paper we discussed the reversible photo triggered volume switching capability of synthesized biocomposite. The photosensitivity of PAAc-co-PAAm [4] were reported by incorporating copper chlorophyllin chromophore into polymer network where, the thermo-responsive volume alteration of chromophore contained polymer was observed. In this work, gold nanoparticles (with varying Au+3 concentrations of 1×10-4 mol/l and 3×10-4 mol/l) have been reinforced into the β-CD modified PAAc-co-PAAm network and visible light responsive volume alteration has been investigated by applying 532nm laser. Both the composites showed 100% solvent release efficiency via reversible positive photo responsivity with zero percentage of memory loss (ML) under pulsatile laser irradiation (Fig. 1). The cytotoxicity study has been confirmed for biocompatibility of the developed polymer composite on L929 mouse breast carcinoma cell line.

Abstract ID: 430
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Composite structural materials
Keywords: Keywords: NASICON-type, Li1.25Hf1.75Al0.25(PO4)3, structural, thermal behavior, ionic conductivity properties

Structural, Thermal and Electrical Conductivity Properties of Al Substitution LiHf2(PO4)3 NASICON-type Ionic Conductor

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Abstract

Lithium ion conducting solid electrolytes, Lithium Aluminum Hafnium Phosphate Li1+xHf2-xAlx(PO4)3 (x = 0 - 0.75) are prepared via solid state synthesis technique. Thermo-gravimetric analysis indicates that the thermal decomposition and thermal stability of the reaction mixture is generally affected by a high content of x substitution. It can be observed that as x content or aluminum substitution increases, the thermal decomposition and thermal stability increases which leads to the sample formation towards higher temperature. For X-ray diffraction analysis, the Rietveld refinement analysis indicates the presence of different types of secondary phases as aluminum content increases. Single phase of Lithium Hafnium Phosphate LiHf2(PO4)3 is only achievable in the absence of any aluminum substitution. Furthermore, for the lithium ionic conductivity, the findings indicate that conductivity increases with increase in x substitution in Li1+xHf2-xAlx(PO4)3. The highest AC conductivity is observable in the sample with composition x = 0.25 of about 2.5 × 10□3 Sm□1 with low activation energy 0.36 eV. The present studies recommend Li1.25Hf1.75Al0.25(PO4)3 to be a future solid electrolyte material for battery applications.

Abstract ID: 431

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: Metal Organic Frameworks, Carbonization, Carbon, Charge and Discharge, Electrochemistry

Metal Organic Frameworks (MOFs) Derived Nanostructures for Electrochemical Energy Storage and Conversion

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MOFs precursors such as MOF-5, Zn-BTC, MOF-199, MIL-101(Cr) and ZIF-12 are converted to pure carbon, and metal oxide decorated carbon structures by the inert-atmosphere template carbonization approach. MOF-derived carbon nanospheres and microporous carbons have delivered specific capacitance in the range of 150 to 350 F g–1, the optimum performance of the designed electrode materials in comparison to the literature. In long-term cycling performance, the copper oxide decorated graphitic carbons and the chromium oxide decorated turbostratic graphitic carbons retained about 95% of their initial capacitance. The novel innovative hybrid composite of cobalt oxide embedded N-doped carbon nanotubes (CNTs) from single-step calcination of ZIF-12 has shown an excellent lithium charge/discharge and storage, retaining ~95% capacity after 50 cycles and a reversible capacity of ~1100 mA h g–1 at a current density of 0.1 A g–1, which far exceeds the performance of conventional lithium ion battery anode materials under similar conditions. Platinum group metal-type (PGM-type) catalysts were deposited on MOF-5-derived high-surface area carbon and electrochemically evaluated for the fuel cell cathodic sluggish oxygen reduction reaction (ORR). The Pt-Ni composition (1:1) exhibited a pronounced positive shift of 90 mV in onset-potential while the Pt-Cu composition (1:1) has delivered an outstanding stability and longevity when evaluated against the commercial Pt/C (20%) catalyst. The significantly improved activity and stability of the catalysts can be attributed to the Pt electron interaction with first-row transition metals and carbon support that prevents the nanoparticles from agglomeration and dissolution as has been proved in X-ray and microscopic analysis.

Abstract ID: 432

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Dielectric materials

Keywords: Millimeter Wave; LTCC; Thermal Efficacity

Interdependency of Dielectric Properties and Temperature for LTCC Material in mmWave Frequency

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The fifth-generation mobile communication system(5G) has a unique feature in employing high-frequency and higher bandwidth for massive data transmission, like everything on cloud, ubiquitous connectivity, intuitive remote access, and immersive experience. Low-Temperature Co-Fire Ceramic(LTCC) technology plays an important role in the fabrication of radio-frequency front end modules for mmWave application, especially in Antenna in Package(AiP) FEM. Understanding temperature dependent performance variation is highly essential for mmWave application. The dielectric constant is attributed to dipole polarization and that depends on the microstructure of the molecules. Structure phase changes and bonding vibration of the crystal unit, caused by the variation in temperature, are prominent factors for change in dielectric constant. Properties evaluation, like dielectric constant, at in-situ temperature and at high frequency is necessary, to provide an estimate of influence of temperature on material properties to the RF designer for designing a circuit or a device structure. In this paper, we designed a Fabry Perot Open Resonator fixture, exposed in a furnace, to measure the variation in dielectric constant and loss tangent between -400C and 1500C in LTCC material. We discussed the relationship between dielectric properties and physical characteristics of the material based on the structure(microstructure), phase change(DSC), and XRD analysis.

Abstract ID: 433

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Carbon and metal oxide based composite materials

Keywords: Graphene oxide, nanocomposites, optical devices

Bandgap Reduction among nanosheets/nanoparticles based nanocomposites of GO/Iron-oxide for optical device fabrications

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Graphene oxide is a promising alternative to Graphene. But the optical bandgap of Graphene oxide is far greater than it is require operating as a semiconductor in electronic devices. In this article we have designed and performed three different schemes to tailor the optical bandgap of Graphene oxide to make it usable in electronic industry. Firstly we have tried to control the oxidation of Graphene oxide during its synthesis. Reason behind this was to control the sp2/sp3 hybridization ratio of carbon. This was achieved with the help of reduced amount of oxidizing agent during its synthesis. Absorption spectrophotometry shows the reduction in optical bandgap of the resultant material as the amount of oxidant is decreased. This decrease in sp2/sp3 hybridization ratio was further confirmed with the help of Raman spectroscopy but this oxidation process is not even throughout the basil plane of graphene oxide flake. X-ray diffraction (XRD) analysis reveals the presence of un-oxidized graphitic domains all over the graphene oxide flake which in turn affects the exfoliation efficiency and hydrophilic properties of the resultant material. Limited range of optical band gap reduction and the reduced exfoliation efficiency caused by the un-oxidized graphitic domains rules out the feasibility of this process. To achieve better range in optical bandgap control another technique is opted that used α-Fe2O3 - Graphene oxide nanocomposite. XRD analysis reveals the in situ reduction of graphene oxide which drastically degrades the crystallinity of graphene oxide by introduction the lattice defects. To overcome this problem a novel synthesis process for Iron oxide-Graphene oxide nanocomposites named as “Wet impregnation method” is devised that uses pre-synthesized Iron oxide nanoparticles. XRD analysis of synthesized nanocomposites rules out the possibility off in situ reduction of graphene oxide. Optical bandgap measured with the help of absorption spectrophotometry reveals the linear decrease in optical bandgap as the loading of Iron oxide nanoparticles is increased from 0.25% to 7%. Morphology of these nanoparticles is probed with scanning electron microscopy (SEM) that rules out all the possibilities of agglomeration of iron oxide nanoparticles and coagulation of Graphene oxide sheets. EDX analysis and Elemental mapping shows the even distribution of iron oxide nanoparticles throughout the Graphene oxide sheets. In the last Raman and Photoluminescence spectroscopy is used to understand the electronic interaction among the constituents of the synthesized nanocomposites.

Abstract ID: 434
Symposium 4: Functional Composite Materials (FCM)
Poster/Oral Presentation
Topics: Nanocomposites
Keywords: Metal, Semiconductor, Hybrid, Nano, Optoelectronic devices.

Ultrafast Hot-electron Transport in Ag-CdTe Hybrid Nanostructure

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The transmission of light through a silver nanocolloid can be changed by irradiating it with an ultrafast pulse. Such transient differential transmission signal recovers in few picosecond timescales which is mainly governed by the electron-phonon thermalization process. In this work, it has been shown that the recovery time of transient differential transmission could be made faster by attaching CdTe quantum dots (QDs) to Ag nanoparticles (NPs). The transient differential transmission was measured at 408 nm and 550 nm by exciting the colloids of bare Ag NP and a hybrid Ag-nCdTe (Ag NP surrounded by 45 CdTe QDs) at 400 nm. In presence of CdTe QDs, the transient differential transmission recovers faster as the probe wavelength is shifted from 408 nm to 550 nm. In bare Ag NPs, the recovery time depends on the temperature of the free-electrons and hotter the electrons more the time for recovery. However, once hybridized, the hot-carriers in Ag NP gets transported to CdTe QDs. This fast transport cools the Ag NP faster. Further, the contribution to the transient differential transmission from CdTe QDs, which has opposite sign to that of Ag NP, reduces the recovery time. Our results are useful in optimizing the hot-electron transport process for faster response in optoelectronic devices and in enhancing photo-detection, energy harvesting and photo-catalytic applications.

Abstract ID: 435

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Sandwich materials/hybrids, Multifunctional composite, Advanced composites

Keywords: Sandwich Laminate, Functionally Graded Core, Three Dimensional Elasticity Solutions, Semi Analytical Approach

Three-Dimensional Elasticity Analysis of Sandwich laminate with FG core by Semi Analytical Approach

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Sandwich panels are used in a variety of engineering applications such as aircraft, construction and transportation where strong, stiff and light structures are required. The major concern in case of sandwich panels is the delamination between core and face-sheets arising from the mismatch of properties between the core and the face sheets. Studies shows that the resistance of sandwich panels to this type of failure can be increased by varying the material properties of the core. Hence the concept of a functionally graded (FG) material is being actively explored in sandwich panel construction.

The accurate analysis of the stresses acting on the transverse planes, which are responsible for delamination is also very important. Only three dimensional (3-D) elasticity theories takes into account all the stresses in the analysis and provide accurate estimate of them. Therefore a 3-D elasticity solution is presented using a mixed semi analytical technique in presented here for a sandwich laminate with FG core.

The sandwich laminate considered here is assumed to be in a state of plane strain. The panel is symmetric with respect to its mid surface. The modulus of elasticity varies exponentially whereas the Poisson's ratio is held constant.

The proposed method makes use of all the equations of 3-D elasticity without making any simplifying assumptions in the formulation, and then the solution is obtained using a numerical integration technique. Further, the proposed approach is based on mixed formulation technique. Thus, the displacements and stresses are evaluated simultaneously with same degree of accuracy. Few examples have been presented to highlight applicability, accuracy and novelty of the method.

Abstract ID: 436

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: TMD, MoSe2, 2D, heterostructures, nano

MoSe2 based Type-II Hybrid nanoheterostructures with different lattice structures for optoelectronic applications

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Transition metal dichalcogenide (TMD) nanosheets with defect-rich and vertically aligned edges are highly advantageous for various catalytic applications. Synthesis of TMDs using the colloidal techniques opens various possibilities to tune the electronic and optical properties of these 2D materials. As an example, we choose MoSe2 nanosheets that have plenty of defects. The defect sites are responsible for adsorption on the surface thereby yielding excellent electrocatalytic hydrogen evolution and other catalytic activities on the surface.

Further, these defects can be employed as seeding points to grow other materials on them. Cu2S in these defect sites leads to a Type-II semiconductor heterojunction that allows for charge separation and therefore the MoSe2-Cu2S forms a superior material for generation of photocurrent.

Further it will be shown that it is possible to form such heterostructures even when large lattice mismatch is present.

Key Words: TMD, MoSe2, 2D, heterostructures, nano

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Abstract ID: 437

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Functionally graded composite materials and structures

Keywords: HOSTs, Lévy's solution, functionally graded plates

Lévy's solution for functionally graded plates using higher-order shear deformation theory

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Equivalent single layer theories (ESL) are extensively used in the analysis of plates. One of the common assumptions that are considered in all the ESL theories is that the thickness is small as compared to the in-plane dimensions. This assumption is the basis for converting a 3D plate problem into a 2D plate problem by considering a displacement-model along the thickness. Higher-order shear deformation theories (HOSTs) consider more realistic non-linear variation of displacements along the thickness as compared to the other ESL theories i.e. classical plate theory (CPT) and first-order shear deformation theories (FOSTs), which consider the linear variation. Due to this reason the solutions obtained using HOSTs are closer to the elasticity solutions. In this paper, static solution of the functionally graded (FG) plates are provided. For FG plates the exponential variation of Young's modulus along the thickness of the beam is considered. Results are obtained for two opposite plate edges having simply-supported boundary condition and other two plate edges having combination of simply-supported, clamped and free boundary conditions. The results obtained are compared with the corresponding results available in the literature.

Abstract ID: 438

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Sandwich materials/hybrids, Multifunctional composite, Advanced composites

Keywords: Sandwich materials, Carbon-fiber tissue, Multifunctional composites, Prepreg process, WiFi antennas

Sandwich-structured composite materials for WiFi antenna application

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In recent years, structurally integrated antennas are growing of interest as the attachment of conventional antennas at the surface of composite material panels impacts their structural integrity [1, 2]. In this study, we investigate a sandwich-structured composite panel made of a honeycomb, E-glass fiber and carbon-fiber pre-impregnated tissues with epoxy resin (prepreg) for WiFi antenna application at 2.45 GHz.

The radiating element is a 35 mm × 35 mm square 370 µm-thick carbon-fiber tissue exhibiting a sheet resistance value Rs = 0.15 Ω/sq. This carbon element is embedded into a sandwich-structured composite material made of E-glass fiber and epoxy resin prepreg tissues (exhibiting dielectric permittivity εr = 5.0 and loss tangent tanδ = 0.01 at 1 GHz) and honeycomb (εr = 1.1 and tanδ < 10-4 at 1 GHz). The carbon radiating element is fed by a carbon microstrip line through a coupled slot in the carbon ground plane (Fig. 1). A reference antenna using plain copper sheets (68 µm-thick and Rs = 2.5×10-4 Ω/sq) for the radiating element, the feeding line and the ground plane has also been fabricated with the same size.

The pattern of both antennas has been designed to operate at 2.45 GHz using a 3-D commercial electromagnetic software. Microwave performance of the carbon sandwich-structured composite antenna has been compared with that of the metal counterpart up to 3 GHz. Measurements of the input impedance, radiation pattern and gain demonstrate the relevance of the carbon-fiber tissues to fabricate a pure sandwich-structured composite antenna for wireless application.

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Abstract ID: 439
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Multifunctional composites
Keywords: Multifunctional composites, Carbon-fiber tissue, Infusion process, Microwave antennas

Carbon composite monopole antenna: fabrication and characterization at microwaves

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Metals are commonly used as radiating elements of antennas. Nevertheless the fabrication process, the weight, and/or the sensitivity to corrosion can restrict their use. Moreover conventional antennas, attached to the surface of composite structures (mainly made of glass-fiber tissues and polyester, vinylester or epoxy resins), can impact the mechanical integrity of such panels. These problems could be circumvented by the development of new composite antennas embedded directly into the composite structures [1].

In this study, we investigate the design, the fabrication and the characterization of a planar lozenge carbon antenna embedded into a composite material panel. To this end, a single ply of a carbon-fiber tissue (woven 2/2, 385 g/m2, 12 K, 370 µm-thick) with a sheet resistance Rs = 0.15 Ω/sq and a square shape (50 mm × 50 mm) acts as the radiating element (Fig. 1). This element has been embedded by infusion process into a 4 mm-thick composite laminate made of E glass-fiber tissue and polyester resin exhibiting dielectric permittivity εr = 4.5 and loss tangent tanδ = 0.01 at 1 GHz. A metal antenna made of a 68 µm-thick plain copper sheet (Rs = 2.5×10-4 Ω/sq) embedded into the same glass-fiber tissue/polyester resin composite laminate has also been fabricated to serve as a reference antenna (Fig. 1). Experimental results, such as input impedance, radiation pattern, and gain of the carbon composite monopole antenna are compared with those of the metal counterpart. Both embedded antennas exhibit microwave performance strictly alike up to 2.1 GHz [2]. A wider discussion will be presented up to 6 GHz.

Accordingly, embedded carbon antennas make them suitable for a lot of wireless applications where smart skins and low profile antennas are required.

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Abstract ID: 440

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: oral bioavailability, peptide drugs, transport mechanism, bile acids target

The bile acids targeted nanoparticles for oral delievery of peptide

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Background: Oral absorption of peptide-loaded nanoparticles is often limited by multiple barriers of the gastrointestinal epithelium. Objective: This study aimed to develop a new drug nanocarrier intended to overcome the barriers associated to the oral modality of peptide administration. Materials and Methods: Hydrophilic glycocholic acid and hydrophobic deoxycholic acid were chose as targets and a novel nanocomplex constituted of low molecular weight protamine - deoxycholic acid and polysialic acid – polyethylene glycol - glycocholic acid will be developed. The mechanism of transmembrane transport, suborganelle localization and targeting in vitro and in vivo of dual bile acid-modified targeted nanoparticles will be elucidated. Results: The nanocomplexes exhibited a unimodal size distribution with a mean size of 145 nm and a negative zeta potential of -19mV, the capacity to associate exentide (~72% association efficiency) and protect it from degradation in simulated intestinal fluids. In Caco-2 cell monolayers, nanocomplexes are internalized via apical sodium-dependent bile acid transporter (ASBT)-mediated endocytosis. The co-localization of FITC labelled nanoparticles and ASBT were visualized in Caco-2 cells. Despite of this, the accumulation of the exentide-loaded nanocomplexes in the distal ileum could be verified in vivo upon their labeling with Cy7. In the overall long-term pharmacodynamic studys of db/db mice, assessed by blood glucose, hemoglobin A1c, body weight, and blood lipid concentrations, of daily oral nanocomplexes (300 μg/kg) for four weeks were equivalent to or better than daily subcutaneous injections of free exenatide solution (20 μg/kg). Conclusion: Based on these results, we provide a scientific basis for the construction of high-efficiency and low-toxicity bile acid modified nanoparticles for oral delivery of peptide.

Abstract ID: 441

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Spintronics

Keywords: Antiferromagnets, Current-induced switching, Domain structure

Current-induced switching in antiferromagnets: role of thermal heating and strain effects

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Possibility of all-electrical switching makes antiferromagnets promising materials for spintronic devices [1-4]. However, recent experiments question the spin-related mechanisms responsible for the switching and elucidate the role of the domain structure [5], heat effects [6-7] and strain [7]. Here we develop a model of switching in antiferromagnets which puts together current-induced temperature gradients, spin-orbit torques, and magnetoelastic effects. Inhomogeneous volume expansion caused by the temperature gradients creates additional stresses whose relaxation induces redistribution of antiferromagnetic domains seen at a macroscopic level as a switching between different states. We calculate the domain patterns and related observable – magnetoresistance, -- as a function of current, and establish equivalence between the values of current and of the magnetic field in switching phenomena. We show that depending on the geometry of electrodes the stress-related mechanism can either compete with or support the switching mediated by spin-orbit torques thus opening new functionalities of spintronic devices. Moreover, high temperature gradient and related stresses can trigger formation of new domain walls and thus substantially change the domain patterns and corresponding macroscopic response. Thus, this study offers a way to optimize efficiency of antiferromagnetic spintronic devices by tailoring of the geometry and proper choice of the constitutive materials.

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Abstract ID: 442

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Graphene, Nano, ZnO nanorods

1D-2D hybrid nanostructures of ZnO nanorods and graphene for next-generation devices

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The demand for photo detector is rapidly growing for a wide range of applications, the potency of one-dimensional semiconductor nanostructures, such as the large surface area versus volume of the nanorods (NRs) [1]. Here we demonstrate the synthesis of 1D-2D hybrid architectures composed of regular arrays of ZnO nanorods formed on graphene. And the fabrication and characterization of new type of high-sensitive photo detecting, composed mainly of vertically well aligned ZnO NRs channel, and graphene - based bottom conductive electrode. Especially for 2D graphene, hybridization with 1D semiconductor nanostructures enables the construction of three dimensional architectures and the imposition of multi functionalities.

Abstract ID: 443

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: MXene, oxidation, synthesis, anti-oxidants

Oxidation and stabilization of 2D MXene nanosheets

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MXenes, such as Ti3C2Tx, are fascinating 2D nanomaterials with an attractive combination of functional properties suitable for applications such as batteries, supercapacitors, and strain sensors. However, practical uses of MXenes, such as Ti3C2Tx, remains challenging as these nanosheets are known to oxidize and degrade quickly from reacting with water and dissolved oxygen. Here, we examine oxidation of MXene nanosheets in various media (air, liquid, and solid) via multiple types of measurements to assess their shelf stability. The oxidation rate of MXene nanosheets were observed fastest in liquid media and slowest in solid media and can be accelerated by exposure to UV light. We also demonstrate an effective method to retard the oxidation of colloidal Ti3C2Tx MXene nanosheets by introducing antioxidants such as sodium L-ascorbate. The success of the method is evident in the conductivity and colloidal stability of Ti3C2Tx. Even in the presence of water and oxygen, the electrical conductivity of Ti3C2Tx nanosheets treated with sodium L-ascorbate was orders of magnitude higher as compared to untreated ones after 21 days. Our findings have the potential to be generalized to protect other types of MXenes (in both the 312 and 211 families) as well and solve the most pressing challenge in the field of MXene engineering.

Abstract ID: 444

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Porous and cellular materials

Keywords: High-internal-phase Pickering emulsion, Porous composite, Polyimide, High thermal diffusivity, Low dielectric constant

Porous boron nitride/polyimide composite films with high thermal diffusivity and low dielectric properties via high internal phase Pickering emulsion method

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This work offers a simple fabrication of porous boron-nitride-(BN)/polyimide-(PI) composite films with high thermal diffusivities and low dielectric constants by combining high-internal-phase Pickering emulsification (HIPPE) and subsequent hot-pressing. BN nanoparticles in composite foams were well dispersed and three-dimensionally connected following the surface of the PI skeleton used as the polymer matrix. The BN contents in the BN/PI composite foams were adjusted in the range of 20–80 wt%. The porosities of the composite films were controlled according to the hot-pressing conditions such as the temperature. The porous BN/PI composite films exhibited high thermal diffusivities of 0.059–1.033 mm2/s and low dielectric constants of 2.08–3.48 at 1 GHz for BN contents of 20–80 wt%. In particular, the BN/PI composite films had extremely low dielectric loss values, close to zero (<0.002) at high frequencies regardless of the BN content and pressing conditions. To the best of our knowledge, no study has reported the use of this method for a BN/PI composite with a high thermal diffusivity and low dielectric constant. These results show the potential of our porous BN/PI composite films as packaging materials with high thermal conductivities and weak dielectric properties for microelectronic devices.

Abstract ID: 445

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Design and application of composite structures

Keywords: replicated composite optics

The Effect of Chemistry and Processing on Quality and Stability of Precision Replicated Composite Optics

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As next-generation space-based telescopes require larger mirrors, replicated composite optics are gaining increased attention due to limitations in the scalability of conventional glass optics. Replication, in this instance, is the process of transferring an optical surface to a thin polymeric film supported by a composite substrate, offering potential weight savings, cost reductions, and faster manufacturing times. For this application, these optical surfaces require both dimensional precision (RMS < 32nm) and dimensional stability in a variety of environments. In previous work, high quality and stability replications have been fabricated with an off-the-shelf UV-cured epoxy resin. The research indicates the behavior is critically dependent on replicating resin material and processing, however, the fundamental properties governing the behavior are not well understood. In this paper, a cycloaliphatic epoxy will be photopolymerized with varying amounts of photoinitiator, modifying the kinetic, mechanical, hygroscopic, and thermal behavior of the replicating resin. Polymer curing behavior and properties, such as moisture absorption and glass transition temperature, are evaluated. By fabricating replications with a range of mechanical, thermal, and kinetic properties, the dominating causes of quality and stability can be understood.

Abstract ID: 446

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Processing and manufacturing technologies

Keywords: Additive manufacturing, natural fibre composite, bioresins

Fabrication of Functional Biocomposites by Additive Manufacturing

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Additive manufacturing or 3D printing is a manufacturing technology which has been introduced during the last 10 years. The technology involves a layer-by-layer build up of a 3 dimensional component, according to a specified geometry and design. Initially the technology was rather marginal, as the obtained components often had a poor quality, low mechanical properties, poor resolution and due to the rather slow production speed. Today the technology has a much better production capacity, and it is possible to process metals, ceramics and plastics by additive manufacturing. Thermoplastic polymers are well suited for the technology, as they can easily be melted and reformed by cooling, and this technology, also named as fused deposit modeling, is now very popular for the production of plastic components.

A challenge for the technology are the mechanical properties, as these are due to the crystallization behavior of the used polymer, which is directly related to thermal transitions the polymer undergoes. It is evident that traditional plastic processing such as injection moulding, will give plastic components with far better mechanical properties than for 3 D printed components. A possibility to improve mechanical properties is to use fibre or textile reinforcements, and structural composites are very important construction materials, especially if low weight and superior mechanical properties are targeted. The integration of textile fabrics and fibres in the 3 D printing process is highly interesting possibility for the production of also large size structural components.

This paper will give an overview of the possibilities to produce composites from thermoplastic polymers and textile reinforcements, by tailoring the 3D printing process. The paper will also report ongoing work with the aim to make biocomposites by using natural fibre reinforcements, which are combined with poly lactic acid as the composite matrix.

The preliminary results indicates that biocomposites with good mechanical properties can be achieved by using the presented concept for producing structural biocomposites. By tailoring the lay-up sequence, as well as the fibre-matrix ratio, it is possible to produce biocomposites with high quality and good mechanical properties. The benefits and advantages for producing biocomposites by 3D printing will be discussed and reviewed, as well as a further ongoing research.

Abstract ID: 447

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Cyanine, J-aggregate, Dye, Alumina, Pseudoisocyanine

Optical Properties of Pseudoisocyanine J-aggregates Embedded in Nanoporous Aluminum Oxide

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Anodic aluminum oxide (AAO) is a self-organized matrix with honeycomb-like structure formed by close-packed arrays parallel cylindrical nanopores (Fig. 1).

The structure of AAO allows the formation of oriented organic molecules, as well as highly organized J-aggregates with unique spectral-optical properties, such as narrower luminescence and absorption spectra in comparison with monomeric forms of dye.

The absorption and luminescence of pseudoiso-cyanine J-aggregates formed in structured cylindrical nanopores of the anodic aluminum ox-ide were studied by the VIS spectroscopy and the laser confocal microscopy.

The luminescence of J-aggregates was observed upon excitation at the absorption J-band as well as at 405 nm. Non-resonant luminescence occurred due to resonance energy transfer from oxygen vacancy in alumina to organic molecules. This is also confirmed by time-resolved luminescence spectroscopy, which shows the increase of luminescence decay time of J-aggregates placed in alumina up to the luminescence time of the clean AAO in comparison with J-aggregates coated on glass substrate.

Such hybrid material can be the basis of advanced optical sensors for atoms and molecules, due to free access of the detected molecules to fluorescent molecular nanoclusters through the nanoporous structure. Owing to the high optical nonlinearity of the organized molecular aggregates, it is possible to develop the optical signal multiplexers. On the basis of AAO activated with dye monomolecules, random lasing was realized, which suggests the possibility of obtaining it also with J-aggregats of cyanine dye.

Abstract ID: 448

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Nanocomposites

Keywords: Nickel Hexacyanoferrate, Nanocomposite, Electrochemical sensing

Preparation of Graphene/Nickel Hexacyanoferrate Nanocomposite for Electrochemical sensing of Ascorbic Acid

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Here we are using Graphene/Nickel hexacyanoferrate (Gr/NiHCF) nanocomposite as a transducer for the first time in electrochemical sensing of Ascorbic Acid (AA). Gr/NiHCF was prepared by mixing equimolar concentration of EDTA containing Nickel nitrate hexahydrate (NiNO3.6H2O) solution into uniformly dispersed Graphene nanoplatelets containing Potassium Hexacyanoferrate (K3FeCN6.6H2O) solution with vigorous stirring. The surface morphology of prepared nanocomposite was studied by using a scanning electron microscope (SEM) and atomic force microscope (AFM). SEM images indicate the uniform deposition of NiHCF on graphene nanoplatelets and confirm the deposited NiHCF particle size is in the range of 50 – 80 nm. Crystallographic and chemical characterization of prepared nanocomposite was done by using X-ray diffractometer, FTIR, Raman, and XPS characterization techniques and it was confirmed that KNiFe(CN)6.xH2O is the chemical structure of deposited NiHCF. Electrochemical characterization of the prepared composite was done by drop-casting Gr/NiHCF nanocomposite ink on the glassy carbon electrode (GCE). The electrochemical performance of the prepared nanocomposite electrode was investigated and compared to the NiHCF compound by using different electrochemical techniques like cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), Tafel analysis and chronoamperometry. All these techniques confirmed the electrochemical activity of prepared nanocomposite was highly efficient and stable as compared to NiHCF. Both, cyclic voltammetry and chronoamperometry techniques confirmed the sensing of ascorbic acid (AA) by oxidizing NiHCF at 0.5 V. Sensitivity (S) and limit of detection (LOD) of prepared nanocomposite electrode towards ascorbic acid was found as 727.2 µA µM-1 mm-2 and 32.54 µM. The interference study proves the fabricated Gr/NiHCF nanocomposite electrode to be a potential candidate for electrochemical sensing of ascorbic acid.

Abstract ID: 449

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Composites, Fine Inclusions, Mechanical Characterization, Image-Based Finite Element Modeling

Image-based Non-segmentation Finite Element Method for Mechanical Characterization of Composite Materials with Fine Inclusions

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Mechanical characterization is an important step in design of new composites and in evaluation of existing materials. Image-based finite element (FE) modeling is a powerful and efficient tool for material characterization, because it requires fewer assumptions compared with the theoretical methods and it is cheaper than the experiment methods. Composite materials with fine inclusions, for example concretes and alloys, are widely used in engineering and industry. To characterize composites with fine inclusions, voxel-based finite element modeling is too expensive especially if the design process is iterative, while a number of challenges arise when the conventional segmentation finite element method is applied [1]. First, segmentation of fine inclusions, if not impossible, is very time consuming; second, segmentation may produce topologically degenerated geometric entities that may not be mesh-able; third, if two inclusions are very close to each other, either severely distorted finite elements will be generated, or very fine elements must be used. To resolve the above challenges, we developed a non-segmentation finite element method based on Riemann sum integration. As suggested by the name, segmentation of inclusions is not required in the method. Numerical examples show that the accuracy of non-segmentation FE model is much higher than segmentation FE model, while its computational efficiency is much higher than voxel-based FE model.

Key Words: Composites, Fine Inclusions, Mechanical Characterization, Image-Based Finite Element Modeling

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Abstract ID: 450
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Bio-inspired design of composites
Keywords: Bioinspiration, nacre, hierarchical structure, stone preservation

Bioinspired nacre-like composites as the next-generation of materials for safeguarding stone heritage

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The fabrication of nacre-like materials by biomimetic mineralization has gained attention as it represents an effective strategy for obtaining materials with outstanding mechanical performance. Taking the microstructure of nacre as inspiration, we are working in the development of a hybrid material composed by highly aligned calcium carbonate (CaCO3) tablets within chitosan and cellulose multilayered films, to obtain continuous hierarchical CaCO3 layers for stone preservation. Particular attention was paid to study the influence of varying layer thicknesses on the interface bonding in samples as well as the effect of surface functionalization of the organic layers (chitosan and cellulose) to modify wettability towards the liquid CaCO3 precursors. Moreover, the application of the developed nacre-like composite as new surface treatments has been studied on marble lithotypes. The main results show that the role of the organic substrate, as well as the use of additives (organic compounds and polymers) are critical to obtain structural control of the mineralized layers, including their orientations, morphology, and hierarchical structure. By controlling the wettability between layers, a better control in the mineralization pathway can be induced. Because of the fracture toughness and mechanical properties of materials can be dramatically enhanced on the nanoscale, this strategy shows a huge potential to be adapted and applied to the stone conservation treatments, extending also their applicability to buildings materials of the future.

Abstract ID: 451

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanomaterials and Nanotechnology

Keywords: Upconversion Nanoparticle; Cicada wing; Photonic substrate; Anti-reflection; Plasmonic Enhancement

Gold Coated Cicada Wings for Plasmon and Anti-Reflection coupled Fluorescence Enhancement in Silica Coated Upconversion Nanoparticles

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Gold Coated Cicada Wings for Plasmon and Anti-Reflection coupled Fluorescence Enhancement in Silica Coated Upconversion Nanoparticles

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Upconversion nanoparticles (UCNPs) are used for bioimaging and multimodal therapies benefiting from their excitation in the infrared (980 nm) and upconverted emission in the visible (400-650 nm). However, the quantum yield (QY) of these UCNPs is <5% limiting their application. Researchers have used various ways to enhance the QY in the UCNPs by plasmons [1], changing the host lattice [1], and using active-core-active shell structures [2]. Recently, we demonstrate that the UCNPs fluoresce 50 times more on a gold (Au) coated Cicada wing. The plasmonic effect arising from the Au coating, coupled with the anti-reflecting (AR) effect of nanostructured Cicada wing substrate is shown for the first time to enhance the fluorescence of the UCNPs dispersed on it. Silica (SiO2) coated Erbium doped green emitting core-shell UCNPs (NaYF4: Yb3+, Er3+@SiO2) show conventional metal enhanced fluorescence (MEF) in presence of plasmonic metals. The plasmon coupling, with an optimally sputtered Au coating, an unprecedented enhancement of >50-fold for the 520, and 655 nm emission of the UCNPs was obtained on the Cicada wings, vis-à-vis planar uncoated (silicon, and quartz) substrates. The enhancement was also confirmed by direct fluorescence imaging of the photonic substrates used. The enhancement in the fluorescence is accompanied by a decrease in the fluorescence lifetime of the UCNPs as predicted by theory.

Keywords: Upconversion Nanoparticle; Cicada wing; Photonic substrate; Anti-reflection; Plasmonic Enhancement.

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Abstract ID: 452

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Experimental methods for Composite materials

Keywords: Zirconium; Nitrides; Plasma processing and deposition; Glow discharge; Surface Hardening

Effect of Nitrogen Gas Ratio and Processing Time on the Properties of Pulsed DC Plasma Nitrided Zirconium

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In the present research, the effect of Nitrogen concentrations (60-90%) in Nitrogen-Argon (N2-Ar) gas admixture plasma and processing time (4, 6, 8, and 12 hours) studies during nitriding of zirconium using 100 Hz pulsed DC Plasma system. X-Ray Diffraction results show the presence of non-stoichiometric Zr3N4 and Zr2N phases with different orientations in the nitride layer. However, the insulating/metastable Zr3N4 phase is dominant in the nitride layer, which indicates the presence of higher nitrogen concentration. The texture coefficient, crystallite size, and residual stresses of the nitride layer vary with the varying concentrations of N2 and the processing time. Surface morphology from optical and scanning electron microscopy indicate the creation of a dense and compact zirconium nitride layer. Electrical resistivity measured by the four-point probe method shows the high value (836 Ω-cm) endorsing the presence of insulating the Zr3N4 phase at higher concentrations. Micro-hardness results show a variation in surface hardness with the variation in the concentration Nitrogen as well as processing time due to the increase of density of the nitride layer. The value of hardness is found nine times higher than that of the untreated surface for the sample nitrided in N2-Ar admixture plasma with a concentration of 70% N2 for the time duration of 12 h. The higher surface hardness is attributed to the denser microstructure and texture coefficient in the nitride layer.

Abstract ID: 453

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Manufacturing and formation techniques

Keywords: Liquid Repellent, Microfluidic Droplets, Springtail Cuticle, Porous Surfaces, Microfluidic Emulsion

Bioinspired and microfluidics-enabled liquid-repellent materials

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Liquid-repellent materials repel liquids instead of allowing droplets to adhere. These materials are important in many fields including self-cleaning clothes and kitchenware, enhanced heat transfer, scald-burns protection, and anti-fouling, anti-corrosive and drag reduction coatings. The dream of research and development on liquid-repellents is a structure that has robust liquid repellency, strong mechanical stability, and is inexpensive to produce on a commercial scale. However, the functional outcomes of existing liquid-repellent materials have not been satisfactory, because of inadequacies of conventional structural design and fabrication approaches in engineering microstructures and properties. We developed a low-cost scalable approach for the fabrication of well-defined porous materials with robust liquid repellency and strong mechanical stability. The design of the liquid-repellent materials is inspired by structures on springtail cuticles, which can effectively resolve the longstanding conflict between the liquid repellency and the mechanical stability. Springtails are soil-dwelling arthropods whose habitats often experience rain and flooding. As a consequence, springtails have evolved cuticles with strong mechanical durability and robust liquid repellency to resist friction from soil particles and to survive in watery environments. We design the porous materials to be composed of interconnected honeycomb-like microcavities with a re-entrant profile: the interconnectivity ensures mechanical stability and the re-entrant structure yields robust liquid repellency. The cuticle-like porous materials are fabricated by self-assembly using microfluidic droplets, which takes full advantage of bottom-up and top-down fabrications and the capabilities of microfluidics in terms of scalability and precise-handling of small fluid volumes. This breakthrough enables inexpensive, commercial-scale production of fluoride-free, durable omniphobic materials that can be made hot-water super-repellent and under-liquid super-repellent as well, and make the dream of no more laundry and no more kitchen-cleaning come true.

Abstract ID: 454

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Theory of graphene, Mxenes and other two-dimensional materials

Keywords: Lamellar zeolites, ZSM-5, Acidity/basicity

A theoretical study of changes in the electronic properties of ZSM-5 zeolite under the transition from bulk 3D to lamellar 2D structure

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As the world's population is continuously growing, the demand for energy, food, and healthcare resources is constantly increasing. In this regard, the challenge facing science and technology is to develop processes for producing sustainable chemicals with low impact on the planet's biosphere. Zeolites are materials that have already shown a significant role in a large number of sustainable processes and even today they continue to represent great innovations. Currently, the latest technology uses nanostructured zeolitic materials, which leads to an improvement in the properties that its analogous represents in bulk. Potential applications of these new materials are in the areas of renewable energy, catalysis, agri-food sector, environmental improvement, sensors, etc [1,2]. Improving the diffusion of molecules within zeolites could boost the catalytic processes that they offer. Particularly, improving the diffusion of molecules within zeolites could increase the catalytic processes that occur in them. This can be achieved in zeolite by reducing its size to the order of nanometers, or by creating flat 2D structures. Although there is no physical obstacle that restricts the production of lamellar zeolites with a nanometric thicknesses, only some of them have been possible to synthesize experimentally, and one of them is known as ZSM-5 [3]. To gain understanding about how the properties of ZSM-5 zeolite are modified when one dimension is reduced to a nanometer size (laminar zeolites), DFT theoretical computations were performed. For the appropriate contrast, the ZSM-5 matrix of purely silica and with an aluminum atom isomorphically substituted in the unit cell were considered for both the bulk and lamellar cases. Additionally, both Na+ and H+ were examined as the exchange cations. The results show that, in contrast to its bulk counterpart, and regardless of the nature of the exchange cation, the conduction band gap for the laminar ZSM-5 zeolite tends to zero. On terms of a population analysis, the acidic/basic character of distinct atoms in various configurations was evaluated. From this analysis, it was found that the acidic/basic character for lamellar zeolite represents an improvement over the respective bulk counterpart.

Abstract ID: 455

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Composite, glass mate, scanning electron microscopy, hand-layup, flexural, tensile

Experimental investigation on mechanical and tribological behavior of epoxy based glass mate reinforced composite

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In current scenario glass fiber-reinforced composite (GFRC) materials are getting more attention because of tremendous mechanical properties and meet the specific needs of a variety of scientific applications. In this paper samples were made by hand-layup manufacturing technique by variations of weight percentage (wt.%) of glass fiber reinforced epoxy composite materials. Fractography techniques were carried out for analysing the fracture surface morphology after performing the tensile test at normal ambience. However compared with pure epoxy resin and found the enhancement in the flexural and tensile strength of the specimens. Although the reduction in wear rate was also noticed with increasing the glass mat content up to 35wt.% and also measured that experimental density of the samples were closed to theoretical density. Moreover, Scanning Electron Microscopy (SEM) was deployed for examined the microstructural characterisation behaviour of GFRC.

Abstract ID: 456

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Fuel Cells

Keywords: Mesoporous N-doped Carbon, ORR Electrocatalyst, Nano, Fuel Cell

Mesoporous N-doped carbon supported Pt nanoparticle electrocatalysts for ORR with enhanced stability and activity

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State-of-the-art support materials for commercial Pt-based PEM fuel cell electrocatalyst are still carbon based (e.g. Vulcan). However, carbon supports suffer from carbon corrosion under long-term electrochemical cycling leading to severe losses in catalyst activity due to Pt particle detachment and eventual electrode collapse. From this point of view, novel support materials for Pt based fuel cell electrocatalysts have to be developed.

In this work, a hard template-assisted synthesis for mesoporous N-doped carbon (MPNC) supports is presented. By this synthesis route a variety of MPNC materials with controlled pore sizes, wall thicknesses, particle size and shapes, as well as N-content and C-sp2 content (in other words graphitization) are accessible. After optimization, the best MPNC material exhibits a higher resistance against carbon corrosion in comparison to Vulcan XC72R, as demonstrated by accelerated stress tests (AST). After Pt nanoparticle deposition by Pt precursor reduction, Pt/MPNC ORR catalyst with higher stability (over 10000 cycles) were obtained when compared to a commercial Pt/C catalyst.

Further, extended heat treatments of the MPNC supports allowed further stability improvements while improved activities were obtained after optimization of the Pt deposition process.

Abstract ID: 457

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Polymeric composites

Keywords: Olefin-Paraffin separation, Metal-organic framework, Mixed matrix membrane, environmental applications.

Pore environment engineering by Metal-Organic Framework (m-Ni-MOF-74) for Ethane-Ethylene separation

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Light olefins are important feed stock in petrochemical industry with an annual demand of 200 million tons. During olefin production, paraffin also produced and its separation is one of the most challenging and energy-intensive processes, which has attracted increasing attention over the past decades. The well-established separation technology in industry, is the cryogenic distillation which requires large distillation columns and required a huge amount of energy. In addition to the traditional cryogenic distillation, non-thermal adsorption separation processes have been developed however regeneration is still an issue. Membrane separation shows great advantages for olefin/paraffin separation due to their low energy consumption, continuous operation and regenerability. Additionally, the rapid development of novel porous materials, e.g., metal-organic frameworks (MOFs) blended in polymers has further boosted the research on the membrane separation of olefins and paraffin in recent years. In this work, we have prepared a porous crystalline MOF-74, and then blended with polyimide polymer. The prepared mixed matrix membrane were tested under the gas permeation setup for Ethane, Ethylene, Propane and Propylene. The developed membrane made of MOF and PI shows the excellent separation of Ethylene from Ethane and Propylene from Propane. The results obtained were compared with the literature which shows the high potential of this membrane in the separation of olefin from Paraffin especially Ethylene from Ethane. Furthermore, this study provide a perspective of the use of other MOFs and COFs in the separation and purification of olefins.

Abstract ID: 458

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Photonic devices and applications

Keywords: conjugated polymer PFO-co-PPV-MEHB; sub-nanoscond TRS, amplified spontaneous emission (ASE) spectra; green emitter

Green Mirror-less laser from Conjugated Polymer (PFO-co-PPV-MEHB) in Film

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The purpose of this work is to investigate the optical and mirror-less laser properties of conjugated polymer (CO) Poly[(9,9-dioctylfluorenyl-2,7-diyl)-co-(1,4-diphenylene-vinylene-2-methoxy-5-{2-ethylhexyloxy}-benzene)] also known as [(PFO-co-PPV-MEHB), ADS125GE], in a thin film. The absorption and fluorescence spectra have been measured at various concentrations in toluene. The amplified Spontaneous Emission (ASE) spectra of CO PFO-co-PPV-MEHB in the thin film have obtained at suitable concentrations and pump energies. The pump source was the third harmonic of Nd: YAG laser (355 nm) in transverse mode. The relationship between input pumping energy and output energy for the samples in solutions has been studied. In addition, the photo-chemical stability of this CO as a laser material was examined. The Time-Resolved Spectroscopy (TRS) studies with the sub-nanosecond resolution have been performed for CO under various pumping energy. These results have provided an understanding of the excited state dynamics of CO PFO-co-PPV-MEHB and have shown that this new CO is quite efficient in the green region under Amplified Spontaneous Emission (ASE) Mode.

Abstract ID: 459

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Anodes and cathodes Materials

Keywords: Glass Cathode, Solid State Battery

A novel, Vanadium containing, mixed conductor glass- a possible new cathode for solid state battery

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Fluoride phosphate based crystalline materials are reported as cathodes for Li ion battery. They offer higher operating voltage due to higher electronegativity and better kinetics due to lower affinity of Li to fluoride anion. However, their direct synthesis is difficult due to rich polymorphism exhibited by A2MPO4F (A = Li, Na; M = Mn, Fe, Co, Ni). Besides, being crystalline, presence of intrinsic spatial voids and channels limit their volumetric energy density. On the other hand, glasses offer advantage of open network structure without porosity, ease of synthesis over wide composition, thereby, fine tuning of properties. Mixed conducting glasses, containing alkali oxide and transition metal oxide, exhibit ionic to mixed conduction with change in composition. Ionic conducting glasses can be used as solid electrolytes, while those exhibiting mixed conduction can be used as cathodes in future version of all solid state battery. Although crystalline fluoride phosphates are reported, literature on glassy cathodes is very limited. To combine the electrochemical advantage of fluoride phosphates and structural, compositional, synthesis advantages of glasses, we fabricated new vitrified compositions in narrow compositional range of LiF–Al(PO3)3 system with addition of Vanadium Oxide. Homogeneous glasses are obtained by melt quenching over wide range of Vanadium oxide content, from 2 to 70 mol%. Glass transition temperature Tg varies between 250–350º C, reducing with increasing Vanadium content, due to decreasing rigidity of glass matrix as it transforms from phosphate to vanadophosphate network. IR spectra reveal that Vanadium acts as network modifier or as second network former depending on its concentration. Changes in glass structure correlate with their measured properties. Room temperature dc conductivity varies from ~10^{-10} S/cm to ~10^{-6} S/cm. Impedance measurements reveal ionic to mixed conduction with changing composition, rendering them as promising glassy cathode material.

Abstract ID: 460

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Photonic devices and applications

Keywords: Vanadium dioxide, Photonic crystal, Distributed Bragg reflector

Transmission control of VO2 nanostructures by IR based 1-D Photonic crystals as hybrid Photonic absorbers

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Effect of 1-D photonic crystals on the optical transmission of VO2 is studied by depositing thin films of VO2 nanoparticles on SiO2/TiO2 distributed Bragg reflectors (DBR) in the near-infrared (IR) spectrum. Monoclinic VO2 nanoparticles with tuned crystallinity were synthesized by a facile solution processing method. Moderately crystalline (MC) and highly crystalline (HC) VO2 nanostructures were obtained by varying its synthesis temperature and post-growth annealing conditions. Both MC VO2 and HC VO2 films exhibit an expected reduction in optical transmission in the IR region due to its structural phase transition from monoclinic (insulator) to rutile (metallic) around a critical temperature of 68 °C. By combining VO2 films on a 50% transmitting DBR structure, the average optical transmission further went down to ~ 15%. The number of stacks of DBR plays a key role in such an effective reduction of optical transmission in IR. When the number of stacks of DBR is further increased from 4 to 7, optical transmission of metallic VO2 films on DBR nearly vanishes in the Near-IR spectrum in such vanadium dioxide/1D photonic crystal based composite photonic structures. Such temperature-controlled, enhanced, broadband optical response can be a promising design for VO2 nanoparticle-based hybrid photonic absorbers for various smart window applications.

Abstract ID: 462

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Functional Magnetic Materials

Keywords: Magnetic nanoparticles, TACE, Clay minerals, Biopolymers

Particle production and characterization for Transcatheter Arterial Chemoembolization applications: comparison of magnetic nanoparticles and clay mineral particles.

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In Transcatheter arterial chemoembolization (TACE) procedure, micron-sized (at least 20 μm) particles and chemotherapeutic agents are injected into arteries that supply oxygen and nutrients to the tumor site. Resulting ischemia and chemotherapy leads to tumor size reduction or necrosis. Arterial embolization is currently performed clinically for the treatment of some cancer types such as liver, kidney tumors yet the particles that are used are mostly polymer beads loaded with chemotherapeutic agents. Multifunctional particles and/or particles with improved drug loading and releasing properties that are also radiopaque, could significantly improve the outcome and increase the efficacy of TACE procedures. In our search for development of improved TACE particles, we used magnetic nanoparticles and clay micro-particles due to their unique properties. Firstly, magnetic micro-particles suitable for TACE applications were produced via bridge flocculation of nanoparticles and drug loading onto their biopolymer coated surfaces. Later clay mineral micro-particles were prepared by loading chemotherapeutic agents and X-ray contrast agents onto their surfaces while controlling their sizes to be applicable TACE applications. Two different structures that are produced were characterized conventionally and in vitro. Furthermore, both produced magnetic micro-particles and clay mineral micro-particles were tested in vivo (rabbit renal model) for embolization and drug delivery efficacy. Results indicated that both structures could achieve embolization, were traceable via X-ray or Magnetic Resonance imaging techniques, and could release drug at the target site. In addition, in vitro cell viability assays carried out for both particles showed no significant toxicity to healthy cells at low concentrations while drug loaded particles behaved like pure forms of the loaded drug against cancer cells. Both particle structures demonstrated specific properties. For example, while magnetic particles enabled magnetic hyperthermia and demonstrated slightly rapid drug release at the target site, clay minerals were biocompatible, possessed extremely high drug loading capacities and significantly extended drug release profiles. These specific properties should be considered before selection of the particles depending on the wanted outcome of TACE procedures.

Abstract ID: 463
Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)
Poster Presentation
Topics: Functional Magnetic Materials
Keywords: Magnetic particles, Biopolymers, Doxorubicin, Drug delivery

Construction and comparison of several different biopolymer coatings on Fe3O4 core-shell nanoparticles produced for Doxorubicin delivery.

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Multifunctional magnetic nanoparticles (MNP) as drug delivery vehicles is a highly researched topic in recent years. Side effects of the used drug could be minimized by accumulating drug loaded MNPs at target site via magnetic manipulations and/or enhanced permeability and retention (EPR) effect. MNPs such as iron oxide nanoparticles (IONP) and their many different formulations are reported to be suitable for drug delivery applications yet there are still several handicaps that needs to be considered such as insufficient accumulation at the target site, toxicity, instability etc. In order to overcome these handicaps, IONPs can be modified to form core-shell structures with biocompatible biopolymers. Biopolymer coatings can modulate physical and chemical properties, improve stability, increase drug loading capacity and optimize drug releasing behavior of IONP core particles. Biopolymer coatings could improve the properties of the core material yet each type of interaction between the drug, polymer and the particle and overall surface charges of core-shell particles could present different outcomes that can affect drug delivery applications. In order to examine these interactions, different types of biopolymers were used to construct Fe3O4 core-shell particles for Doxorubicin (DOX) delivery. Polymers were selected depending on their biocompatibility, ionic charges and thermal behaviors. Hydroxyl ethylene cellulose (HEC), nanocrystalline cellulose (NCC), a synthetic biopolymer polyvinyl pyrrolidone (PVP) and □-Carrageenan (□-CA) were selected for this study. Fe3O4 nanoparticles were coated with each polymer with various concentrations in order to obtain the proper concentrations. Most suitable concentrations were determined via Zeta potential, dynamic light scattering measurements and rheological analysis. Later, for the chosen biopolymer concentrations Fe3O4 core-shell particles were further characterized by conventional and in vitro methods. DOX loading capacity determination, in vitro cell viability and drug releasing assays were carried out for every Fe3O4 core-shell particle. The results obtained from this study indicated that HEC coated Fe3O4 core-shell particle formulation was the most suitable for DOX delivery applications because HEC (a cationic biopolymer) achieved full coverage of the core surface, reduced toxicity to normal cells and successfully loaded and released DOX. On a side note, □-CA could be a better candidate if the method of drug delivery includes inducing magnetic hyperthermia due to thermo-responsive nature of the polymer, even though the □-CA coatings displayed decreased drug loading capacities.

Abstract ID: 464

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Composite structural materials

Keywords: FCFDT, Inside-outside Diameter Ratio, Flexural-shear Strength, SMA

Structural Behavior of Fiber Concrete-filled Double Skin Steel Tubular Beams Subjected to Monotonic Bending

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Construction materials for buildings in the future are expected to have diverse forms and types, thus contributing to the emergence of new multifunctional buildings. Various types of materials are currently being developed, but it is difficult to find examples of buildings that actively use shape memory alloys (SMAs), fiber materials (Steel Fiber, Nylon) and fiber concrete-filled double-skin steel tubular (hereinafter, FCFDT). FCFDT members are made of two steel pipes with different diameters placed in concentric squares and filled with concrete between the two steel tubes. This paper examines the structural behavior of the FCFDT fabricated with the installation of reinforcement bars and SMAs in the inner and outer steel tubes, the concrete strength, the fibers, and the inner-outer diameter ratio (Di/Do) as the main variables under the monotonic bending. This work compares the existing reference formula for flexural-shear strength with test result to provide the basic data for the design of the FCFDT beams. Towards this end, the load-deflection relationship, the failure type, flexural-shear strength, and displacement ductility were compared and analyzed. The results of this study confirmed that the appropriate use of SMAs and fibers can improve the shortcomings associated with steel tube such as brittle fracture behavior.

Abstract ID: 465

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: UHMWPE, SBA-15, Nanocomposites, Mechanical performance

Disentangled UHMWPE and UHMWPE/SBA-15 nanocomposiites with improved processability and excellent mechanical performance

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Ultra-High Molecular Weight Polyethylene (UHMWPE) shows high wear and fatigue resistances and superior impact toughness and a high biocompatibility allowing its use for orthopedic and cardiovascular implants. The medical segment is one of the primary markets accounting for almost 30% of market share in 2016, but UHMWPE is also used for many other industrial applications. Despite the success of the prosthetic devices some problems still prevail regarding wear of UHMWPE component. Another limitation is the poor processability of UHMWPE and the high energetic costs associated1.

This work intends to provide a contribution to the two above mentioned problems and proposes the development of a new processing methodology for disentangled UHMWPE nascent powders along with the preparation of UHMWPE composites containing SBA-15 particles. A simple approach based on compression molding is proposed involving high pressure and a processing temperature below the main melting peak. The obtainment of disentangled chains in the nascent powders during polymerization is achieved, by using a "quasi-living" bis [N-(3-tert-butylsalicylidene) pentafluoroanilinate] titanium(IV) dichloride (FI) catalyst under selected conditions. The UHMWPE nascent powders and the corresponding films obtained by compression molding, at optimized temperature and pressure conditions, show very high melting temperatures (139,5 ºC < Tm < 141,5 ºC) and crystallinity values (0,73 < fc < 0,80) supporting the existence of a disentangled state. These high crystalline UHMWPE based materials show an extraordinary increase of the indentation modulus (~330%) and of the hardness at surface (~250%), when applying the proposed methodology to the nascent UHMWPE prepared in homogeneous conditions. Still higher mechanical performance can be achieved for UHMWPE/SBA-15 nanocomposites obtained when mesoporous SBA-15 particles are used as catalyst carrier and filler during polymerization. Moreover, the methodology used for the immobilization of the catalyst was also found to affect the reinforcement effect of SBA-15. A simple and economic solvent-free approach has been developed for disentangled UHMWPE processing.

Abstract ID: 466

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Metamaterials and Materials for THz, Plasmonics and Polaritons

Keywords: Terahertz, TMDs, Modulation depth

Optically Controlled Modulation of Terahertz beam using few layers of Group 5 TMD-TaS2 on Silicon

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The Terahertz (THz) modulator based on group 5 layered TMDs material tantalum sulfide (TaS2) is demonstrated by incorporating the TaS2 thin film on the high-resistivity silicon substrate. The THz transmission is optically controlled by using continuous laser irradiation with a maximum power of 1W/cm2. The transmission spectra are measured in the THz frequency range from 0.1-0.5 THz by using a continuous-wave frequency-domain THz measurement system. It has been observed that THz transmission decreases with a gradual increase in laser power. The reason is the change in conductivity because of photogenerated charge carriers which result in attenuation of the THz beam. Under low pumping power of 1 W/cm2, the modulation depth of 59.7%, 58.4%, at 0.2 THz and 0.5 THz frequency respectively is achieved. The transition metal di-chalcogenides based modulators can be effectively utilized in the wide variety of THz fields such as communication, imaging, and spectroscopy.

Abstract ID: 467

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Functional Magnetic Materials

Keywords: Multiferroics, Magnetoelectrics, Magnetic Properties, Dielectric Properties, Optical properties

Effects of lattice disorder generated due to A–site size variance between Bi3+ and RE3+ (RE = Nd3+, La3+, Gd3+, Dy3+) cations in BiFeO3

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Effects of lattice disorder generated due to A–site size variance between Bi3+ and RE3+ (RE = Nd3+, La3+, Gd3+, Dy3+) cations in BiFeO3

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Lattice disorder effects due to A–site size variance between Bi3+ and RE3+ (RE = Nd3+, La3+, Gd3+, Dy3+) cations in BiFeO3 (BFO) have been substituted with fixed 10% RE3+–ion concentration. All the system showed a partial structural transformation from orthorhombic to R3c phase as confirmed from Rietveld refinement of X-ray diffraction data. Reduced tolerance factor values for rare earth doped systems indicate the coexistence of both in–phase and anti–phase tilting system. A significant destabilization of FeO6 octahedron has been observed as suggested by softening of phonon modes corresponding to oxygen motion. Optical studies performed in the spectral range from 1.5 eV to 5 eV showed three charge transfer transitions and a doubly degenerate d–d transition. A red shift observed in d-d transition energies which is an indication of variation in crystal field splitting. Weak ferromagnetism in all RE3+ doped samples has been observed which is ascribed to the suppression of the spiral spin structure inherent in un-doped BFO. The variation in magnetization in different systems is also related to the changes in Fe-O-Fe bond angle (confirmed from Rietveld refinement) due to the strain induced in the unit cell by RE ions. The temperature dependent dielectric studies show an increase in dielectric constant with increase in temperature (typical behavior of ferroelectric below Tc). However, no dielectric anomaly corresponding to ferroelectric to para-electric transition has been observed indicating that transition temperatures lie above the studied temperature window.

Keywords: Multiferroics, Magnetoelectrics, Magnetic Properties, Dielectric Properties, Optical properties

Abstract ID: 468

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Thin Films and Nanomagnets

Keywords: Color filter, Multilayer film, silver, zinc sulfide, UV–vis spectroscopy

Fabrication of Ultrathin Artificially Stacked Ag/ZnS/Ag Multilayer Films for Color Filter Applications

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A novel strategy for the fabrication of mechanically and thermally stable highly efficient resonant structure assisted ultrathin artificially stacked Ag/ZnS/Ag multilayer films on cleaned glass substrates using thermal evaporation technique are demonstrated. These multilayers have good adhesion to each other and to the glass substrate, resulting in mechanical and thermal stability. The results of the structural analysis, surface morphology and atomic force microscopy of these filters confirm the good crystallinity with a low value of surface roughness. The effect of thickness of artificially stacked metal (Ag) and dielectric (ZnS) layers has been examined in terms of optical properties by several spectroscopic techniques. These ingenious filters exhibit a large and deep stop band in the visible wavelength region. Thus blue, green and red color filters, centered at 460, 540 and 620 nm having bandwidths of about 25, 44 and 35 nm, respectively, were achieved. Moreover, the statistical outcomes of all the three filters (blue, green and red) show that the peak transmission efficiencies are consistently 73%, 70% and 63%, respectively. Additionally, the effect of different angles of incidence on the transmittance spectra has also been presented. Hence, the obtained results strongly suggest that these filters can be potentially used for tuning the color of optical filters according to the desired applications.

Abstract ID: 469

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Functional Magnetic Materials

Keywords: Thin Film, Pulsed Laser Deposition, Magnetization

Spin state dependence on oxygen content in SrCoO3-□ thin films

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Strontium cobaltates (SCO) is observed to be a fascinating material due to its topo tactic phase transition from brownmillerite (BM) SrCoO2.5 to perovskite (P) SrCoO3. It is reported that there is a high spin to intermediate spin transition as one moves from SrCoO2.5 to SrCoO3 [1,2]. However, a systematic study on the variation of spin state with oxygen content is not yet reported. In the present paper, we have studied the magnetization measurements of SCO thin films with different oxygen content to find out the correlation of spin state with oxygen content.

We have grown a 70 nm thick film of SrCoO2.5 on single crystal SrTiO3 (STO) (001) substrate by PLD. We cut the film into three pieces and dip it into NaClO solution for a different duration (E1: 6 min, E2: 15 min and E3: 21 min) to oxidize and obtain its structure close to SrCoO3. Structural characterization of all the films were carried out by X-ray diffractometer while magnetic properties were measured by 7-Tesla SVSM (Quantum Design). X-ray diffraction (XRD) study reveals that all the films are of perovskite (P) phase with coexisting tetragonal and cubic phase corresponding to different oxygen content as measured from area ratio of both the phases [2,3]. The crystal field at the Co ions are different for tetragonal and cubic phases which causes difference in spin state and the Curie temperature. Moving from E1 to E3 tetragonal phase fraction reduces and cubic phase fraction increases which implies an increase in oxygen content. Magnetization versus temperature (M-T) in both Field Cooled (FC) and Zero Field Cooled (ZFC) cycles and magnetization versus field (M-H) measurements of E1, E2, and E3 films shows ferromagnetic nature with Curie temperature 273 K, 269 K, and 266 K and saturation magnetization 1.93□□□/f.u., 1.34□□□/f.u., and 0.91□□□/f.u respectively. Further, Curie-Wiess fitting confirmed that the change in oxygen content changes the local crystal symmetry which leads to modify the spin state and the Curie temperature. Thus, we conclude that the oxygen content influences the spin state and the Curie temperature of the SCO thin films.

Abstract ID: 470
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Nanocomposites
Keywords: Graphene, ZnO, Nanocomposite, Xanthine, Biosensor.

Electrochemical xanthine biosensor based on Reduced Graphene Oxide-Zinc oxide Nanocomposite

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Fresh meat, being rich in nutritional value, is required in food industry for manufacturing of high-quality products. Keeping the freshness of meat on an acceptable quality level is highly desirable in food industry to manufacture safe and qualified products. The high concentration of various enzymes results in spoilage of freshness of meat. Among various enzymes, Xanthine (Xn) is one of the decomposing products responsible for meat spoilage. The conventional techniques for the detection of Xn is costly, time-consuming, and lead to toxic end-waste products. So, to overcome these limitations, there is an urgent need for the development of biosensors.

Herein, we report an electrochemical Xn biosensor based on covalent immobilization of xanthine oxidase (XO) onto reduced graphene oxide-zinc oxide (rGO-ZnO) nanocomposite. The rGO-ZnO nanocomposite was synthesized using the hydrothermal method and was electrophoretically deposited on indium tin oxide (ITO) coated glass substrate at optimized conditions. The nanocomposite was characterized using X-ray diffraction, scanning electron microscopy, UV-visible and Fourier transform infrared spectroscopy. The fabricated bioelectrode has been used for the detection of Xn using differential pulse voltammetry and cyclic voltammetry. Efforts have also been made to validate the fabricated biosensor with real samples obtained from the fish. Furthermore, the synthesized biosensor showed good selectivity, reproducibility, and has the potential to be used to detect the freshness of meat.

Abstract ID: 471

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: Self-standing CNT, MoS2-CNT hybrid, Heterostructures, Magnetron sputtering, Supercapacitor

Free-standing hydrophilic carbon nanotube films supported edge exposed MoS2 nanoflakes for flexible supercapacitor application

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Recently, two-dimensional layered structures, specially MoS2 has come out as the most investigated electrode material for batteries and supercapacitors, possessing well preserved in-plane covalent bonding, leading to extraordinary mechanical elasticity within the layers as well as outstanding firmness along the c-axis. The present work is aimed to fabricate vertically aligned edge exposed molybdenum disulfide nanoflakes on the surface of the self-standing hydrophilic carbon nanotubes, using a two-step process involving a chemical route and magnetron sputtering techniques for flexible supercapacitor application. These hybrid heterostructures have been characterized using XRD, FESEM, TEM, XPS and cyclic voltammetry. The three electrode measurements revealed very high areal capacitance of 0.2 F/cm2 at a scan rate of 10 mV/sec in 1M Na2SO4 system. The electrode was then tested for 3000 cycles (50 mV/sec), in which the system displayed extraordinary capacitance retention of 99.2%. Next, we constructed a symmetric supercapacitor device using MoS2-CNT hybrid heterostructures and found enhanced electrochemical performance with energy density of the order of 400 μW h/cm2. Also, the bending measurements revealed that the device capacitance as well as the charging-discharging rates had no major influence, indicative of robustness of our device. The inherit hydrophilicity and controlled chirality of carbon nanotubes makes them an ideal candidate for electrode material. Moreover, their self-standing nature allows them to function both as the active material, as well as highly conductive current collector. Coherent and efficient design of structurally stable electrodes is very significant, when aimed at high-performance flexible electrochemical energy storage devices.

Abstract ID: 472

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Advances in electrolyte and electrolyte additives

Keywords: Conducting Polymer, Gel Electrolyte, Energy Storage

Functional Gel Electrolyte for Concurrent Solar Energy Harvesting and Charge Storage

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Due to the intermittent nature of solar energy, energy storage is essential in electronic devices which are powered by harvesting solar energy. Both solar cells and energy storage elements (i.e. batteries or supercapacitors) are relatively large components and occupy a significant amount of space in a small electronic device such as a wireless sensor. Composite gel electrolyte materials made from a conducting polymer (i.e., Polyaniline) and a dye (e.g., Methylene Blue) have presented unique properties of photogeneration of electric charges and charge storage in the bulk electrolyte that was employed for making photoactive supercapacitors. The electrical and optical properties of the gel at various concentrations of the conducting polymer and the impact of that on the energy harvesting and charge storage in a two-terminal photoactive supercapacitor have been studied. It is found that a simple device made from a TiO2 coated conductive glass/gel/porous carbon electrode has a specific capacitance of 863 mF/g and can be charged with a solar simulated light (80 mW/cm2) up to 140 mV. The fabricated device showed a charge storage stability higher than 2 hours. The mechanism of internal charge storage is believed to be due to the photoredox reaction in the conducting polymer. Further development of the composite gel can address the need for making compact devices with the dual properties of enrgy harvesting and storage.

Abstract ID: 473

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Carbon and metal oxide based composite materials

Keywords: Nickel Oxide, Carbonaceous template, Multi-shells, Electrochromism, Glucose sensing

Multi-shelled Nickel oxide hollow-microspheres as bifunctional material for Electrochromic smart window and Non-enzymatic glucose sensor

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Nickel oxide (NiO) has been considered as one of the most promising candidates among various transition metal oxides due to its natural abundance, excellent electrochemical performances and obviously due to its environmentally benign nature. It has been observed that the morphology of a material plays a crucial role to upgrade its overall electrochemical properties, improving the kinetics of ion/electron exchange reactions. In this work, we obtained a facile hydrothermal route for the synthesis of NiO multi-shelled hollow microspheres. Here, carbonaceous saccharide microspheres had been used as sacrificial template to the formation of multi shells of NiO hollow microspheres. The multi-shells of the hollow spheres provide enhanced active surface area and additional reactive sites, which facilitate the faster ion intercalation and deintercalation, play key role in glucose sensing and electrochromism. This study offers a promising route to design advanced electrode materials for electrochromic smart windows and non-enzymatic glucose sensors.

Abstract ID: 474

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster/Oral Presentation

Topics: Theory of graphene, Mxenes and other two-dimensional materials

Keywords: Transition metal dichalcogenide (TMD), edge effects, nonradiative lifetime

Edge effects for nonradiative recombination in WS2

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Transition metal dichalcogenide (TMD) monolayers with direct band gaps are promising materials for various electronic and optoelectronic application. Understanding edge effects and quantifying their influence on the carrier lifetime of monolayer TMDs is fundamental for applying them to high performance electronic and optoelectronic devices. Monolayer WS2 (tungsten disulfide) with higher photoluminescence quantum yield than other two-dimensional semiconductors (e.g. MoS2) suggesting relatively low defect density. However, the edge can contain a high density of dangling bonds that can affect the carrier lifetime. Here, we build several possible monolayer WS2 edge models to simulate edge effects for nonradiative lifetime in monolayer WS2. These edges introducing trap states into the system can adjust the nonradiative lifetime because of different mechanisms. We are also trying to develop models that quantify the relationship between the nonradiative lifetime and the ratio of the number edge atoms to the number of all the atoms in the model. This study provides a reference for the practical design considering the edge effects for the lifetime of electronic and optoelectronic devices using TMDs from a theoretical perspective.

Abstract ID: 475

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Sandwich materials/hybrids, Multifunctional composite, Advanced composites

Keywords: Metal Organic Frameworks, MOFs, Nanoparticles, Composites, Photoreduction, Carbon dioxide, and Energy Conversion

Cu2O@MOF Composite as a Highly Efficient Catalyst for Carbon Dioxide Photoreduction

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Carbon dioxide conversion into value-added products has attracted great interest as an alternative sustainable approach to mitigate CO2 emissions and its global environmental problems, such as the greenhouse effect. In recent years, Metal-Organic Frameworks (MOFs) photocatalysts have shown a remarkable promise in the photoreduction of CO2. Herein, a novel photocatalytic composite based on NH2-MIL-125(Ti) and copper oxide (Cu2O@NH2-MIL-125) was developed through in situ growth of the MOFs crystals around the Cu2O nanoparticles with different ratios. The obtained materials were structurally characterized using powder X-ray diffraction. The photophysical properties of the pristine MOFs and their composites were studied using various spectroscopic techniques. The experimental results showed that formate was the main CO2 reduction product, and it also revealed the superiority of Cu2O@NH2-MIL-125 over the pristine MIL-125 in the conversion activity. The high photoactivity of Cu2O@NH2-MIL-125 can be attributed to the effective concentration of CO2 within the pores of the MOF around the Cu2O, and the transfer of photo-induced carriers from the MOFs into the Cu2O nanoparticles.

Abstract ID: 476
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Bio-composites
Keywords: Electrospinning, Hydra CPP-1 and Cnidoin, Cross-linker free nanofiber

New Class of Crosslinker-Free Nanofiber Biomaterials from Hydra Nematocyst Proteins

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Nematocysts, the stinging organelles of cnidarians, have remarkable mechanical properties. Hydra nematocyst capsules undergo volume changes of 50% during their explosive exocytosis and withstand osmotic pressures of beyond 100 bar. Recently, two novel protein components comprising the nematocyst capsule wall in Hydra were identified. The cnidarian proline-rich protein 1 (CPP-1), characterized by a “rigid” polyproline motif, and the elastic Cnidoin possessing a silk-like domain were shown to be part of the capsule structure via short cysteine-rich domains that spontaneously crosslink the proteins via disulfide bonds. In this study, recombinant Cnidoin and CPP-1 are expressed in E. coli and the elastic modulus of spontaneously crosslinked bulk proteins is compared to that of isolated nematocysts. For the fabrication of uniform protein nanofibers by electrospinning, the preparative conditions are systematically optimized. Both fibers remain stable even after rigorous washing and immersion into bulk water owing to the simultaneous crosslinking of cysteine-rich domains. This makes our nanofibers clearly different from other protein nanofibers that are not stable without chemical crosslinkers. Following the quantitative assessment of mechanical properties, the potential of Cnidoin and CPP-1 nanofibers is examined in relation to the maintenance of human mesenchymal stem cells.

Abstract ID: 477

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Electrical properties of graphene, Mxenes and other two-dimensional materials

Keywords: Molybdenum Disulfide, Intrinsic Scattering, Field-Effect Transistor

Intrinsic Impurity Scattering in The Two-Dimensional Channel Material of MoS2

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Two-dimensional (2D) materials such as MoS2 are natively sheet of one atomic thick. They are free from dangling bonds that cause unstable surface for three-dimensional (3D) materials with a reduced thickness. In particular, it is demonstrated that these 2D materials usually present a high on/off ratio, a high mobility, and a debased short channel effects for field-effect transistor (FET) applications. As for their applications in channel materials, the novel 2D materials, however, have not been explored in detail yet. Here we present a systematic study of the intrinsic impurity in the 2D material of MoS2. We use mechanical exfoliation to disperse 2D MoS2 flakes on silicon wafer capped with a 300-nm thick SiO2 layer. The standard electron-beam lithography and thermal evaporation are used to pattern metal electrodes on the top of the MoS2 flakes as source and drain electrodes. With the back gate electrode from the heavily-doped silicon substrate, the MoS2 FET devices are investigated for the study of device performance such as the on/off ratio, the mobility, the substhreshold swing, and the interface trap density. In our studies, we especially focus on electron transport measurements thus we study temperature dependent behaviors from 300 K down to 80 K. We apply Mott's 2D variable range hopping transport to analyze electron transport. In our results, we will show that each exfoliated MoS2 flakes, even obtained from the same bulk, will display completely different intrinsic impurities. We therefore recommend to explore the contact or the substrate effects by using the same flake. The MoS2 flakes sometimes show low mobility and sometimes present high mobility. For those of high-mobility flakes, we always discover a metallic state at a high carrier concentration. All our results point to the truth that, for the MoS2 flake with a high-crystalline quality, the mobility is always higher than 50 cm2/V s. For those high mobility flakes, we observe an insulator to metal transition at a high carrier concentration and the mobility increases with decreasing temperatures. The study confirms that high quality MoS2 can be used for the application of FET channel materials.

Abstract ID: 478

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Industrial applications of composite materials

Keywords: superconducting magnetic separation, environment remediation, material resource, circular economy

The materialprocessing with superconducting magnetic separation for Circular Economy

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The magnetic separation technology has many features due to its physical treatment:

1. The simple and flexible equipment system from the small to the large scales

2. The stable and fast treatment

3. Few chemical change after treatment

4. Few secondary waste production after treatment

The magnetic separation technology is supported by the magnetic force Fm as shown in equation (1).

$$Fm = Vp \cdot M^* \cdot \mu_0 \nabla H \quad [N] = \chi_{eff} \mu_0 Vp \cdot H \cdot \nabla H \quad [N] \quad (1)$$

The key components of Fm are Magnetic seeding (related parameter χ_{eff}) or Magneto-Archimedes effect(χ_{eff}), Aggregation (Vp), Magnetic field (H) and its gradient (∇H) .

The strong magnetic field affect the key components directly or indirectly and increase Fm. The material processing with superconducting magnetic separation SMS technology is applicable to ferromagnetic, paramagnetic and diamagnetic substances. The SMS technology dramatically developed the application for environment remediation and material resource.

The developed SMS technologies are increasingly important to realize Circular Economy by contribution 3R(Reuse, Recycle and Reduce) execution.

The SMS projects started from around 1995 in Japan. The R & D has been continued since that time. The technical reports were published and the annual conference session has been opened in Japan.The IFMFC (International Forum of Magnetic Force Control) started in 2010 at the call of Japanese researchers to Korean and Chinese researchers and opened every year .

The application of SMS technology developed to the harmless waste production, the raw

material production, energy saving, volume reduction of Cs contaminated soil and so on.

Key Words: Superconducting magnetic separation, Environment remediation, Material resource, Circular Economy

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Abstract ID: 479

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Optical properties of metals and non-metals

Keywords: TRS, Conjugated oligomer BHFT, excimer, amplified spontaneous emission spectra.

Time Resolved Dynamics of Dual Amplified Spontaneous Emission (ASE) from an conjugated oligomer 3,7-Bis-(9,9-di-n-hexylfluoren-2-yl)-dibenzothiophene-S,S-dioxide in solution

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The laser action from a conductive oligomer 3,7-Bis-(9,9-di-n-hexylfluoren-2-yl)-dibenzothiophene-S,S-dioxide (BHFT) has been demonstrated in this study. First absorption spectra were studied for BHFT in Toluene under a wide range of concentrations. The spectra showed that there was only one peak at 355 nm under a wide range of concentrations indicating the absence of dimerization. The fluorescence spectra for low concentrations showed two peaks, at 395 nm and 415 nm, which could be attributed to the monomer and the excimer. At higher concentrations, the peak at 395 nm almost vanished and the dominant peak was at 415 nm with a hump at 435 nm. Laser action was tested in a transverse pumping configuration where the conducting oligomer was pumped by laser pulses from the third harmonic of an Nd:YAG laser (355 nm). It could be seen that there were dual amplified spontaneous emission (ASE) peaks, at 395 and 415 nm. These peaks could be attributed to the V1 and V2 vibronic band of the BHFT oligomer; but, even after our best efforts, we were not able to observe the ASE peak at 435 nm corresponding to the hump in the fluorescence spectra. The power of ASE and the photochemical stability were remarkably high. This trend for the oligomer is entirely different from its conjugated oligomer BECV-DHF and similar to HOTF. The Time-Resolved Spectra (TRS) shows the formation and kinetic competition between two vibronic bands V1 and V2. This is perhaps the first report on TRS dynamics of dual ASE from vibronic states of the conjugated oligomer BHFT in liquid solutions.

Abstract ID: 480
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Bio-composites
Keywords: blood platelet, collisions, aggregation

Aggregation Dynamics of Particulate Blood Platelets

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Abstract

Blood is not only the first contact for nanoparticles (NPs) administered intravenously, but also the gateway for all NPs, administered via other routes, to reach their target tissues or organs. The size of NPs allows them to easily distribute throughout the body, traverse biological barriers and enter the systemic circulation where they can readily penetrate cells [1]. The size of NPs also makes them more biologically active than micro-sized particles, allowing disruption of the normal cellular biochemical environment. NP interactions with blood components is, therefore, not only inevitable but also potentially perilous and hemocompatibility should be one of the foremost concerns in the design and development of NPs with therapeutic applications

Blood is a complex fluid which is a suspension of red blood cells (RBC) or erythrocytes, white blood

cells (leukocytes), and platelets in aqueous solution of proteins and salts (plasma). Platelet aggregation at sites of vascular injury is necessary for hemostasis and arterial thrombosis and occurs via platelet–platelet adhesion, tethering and rolling on the injured endothelium, a critical initial step in blood clot formation. In straight vessels, the presence of erythrocytes, red blood cells (RBCs) is known to push platelets toward walls, which may affect platelet aggregation and thrombus formation. The effects of RBC collisions, RBC aggregation, RBC deformability, RBC cytoplasm viscosity, platelet size and shape, platelet adhesion forces, and channel size on platelet margination, shear forces on platelets, and the process of thrombus formation is done by tracking individual cells through computational simulation.

In the presence of RBCs however, mural thrombus mass was found larger in the highly tortuous arteriole compared to the less tortuous arteriole. Smaller platelet size yielded less mural thrombus mass and smaller emboli, either with or without RBCs. Aggregation of platelets is accelerated by shear rate during blood flow. The adhesion of platelets to each other and to Red Blood cells depend on collisions of elastic platelets to soft RBC in a hydrodynamic flow with Johnson-Kendall-Roberts (JKR) models In this way the cohesive impulse, required for the hard-sphere model, is calculated together with other parameters, namely the collision duration and the coefficient of restitution. Aggregate morphology, elastic modulus and surface energy are critical in determining adhesion to straight and tortuous capillary walls and to Red Blood Cells for required optimizing coagulation. Model predictions on platelet to platelet collisions and of platelets to the capillary wall showed that platelet size, platelet Young's modulus and shear rate are most significant variables controlling capillary aggregation and thrombus. The role of nanoparticles in affecting collision and aggregation of platelets is discussed.

Abstract ID: 481

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Spin waves and magnonics

Keywords: Multiferroics, Spin-waves, Far infrared spectroscopy

Suppression of Spin wave excitations in BiFeO3 at low temperature

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Bismuth ferrite (BiFeO3) is a room temperature multiferroic exhibiting simultaneous ferroelectric and magnetic orders. Its G-type antiferromagnetic order is modulated with a cycloidal spin structure having a wavelength of 62 nm. Further, its magnetic structure is reported to show soft ferromagnetic behavior at low temperatures and undergoes two spin reorientation transitions at 250 K and 150 K.

In this study, we report on the Far-IR reflectivity measurements carried out on BiFeO3 pellets using Bruker Vertex 80v FTIR spectrometer. We have detected eleven SWEs at room temperature (see Fig. 1a). Six of them are assigned to extracyclon (□) modes (see Fig. 1b). The remaining five SWEs are assigned to cyclon (□) modes (see Fig. 1b). The cyclon mode □10 is absent at room temperature. The frequencies of extracyclon and cyclon modes are fitted with the equations E_exc=(n^2+1)^(1/2) □_c and E_exc=n□_c respectively, where □c is cyclon energy. The cyclon energy as determined from the fits is found to be 5.8□0.2 cm-1, which is close to the theoretical value of 5.3 cm-1 [1]. The behavior of these SWE modes has further been followed with decreasing temperature. It is observed that the SWEs modes are getting suppressed at low temperatures (see Figs 1a and 2b), which indicates a destruction of spin cycloid down the temperature. This is also evident from enhancement of soft ferromagnetic behavior down the temperature. On the other hand, the □10 cyclon at 56.7 cm-1 starts emerging below 250 K (Figs. 2a and 2b). This mode is reported to be an electromagnon [2]. Thus, we see an improvement in magneto-electric coupling at low temperatures as the integrated intensity of the □10 mode is increasing contrary to other SWEs.

Abstract ID: 482

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Piezotronics for smart systems

Keywords: BaTiO3/ PDMS composite, ZnO, GO, PEDOT:PSS, Piezo energy harvesting

Piezoelectric response of BaTiO3/ PDMS composite on incorporation of ZnO, GO and PEDOT:PSS with different doping concentrations and at different temperatures

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Lead free Flexible piezoelectric sheets are found suitable for the fabrication of biomedical piezoelectric devices. We made a lead free Piezo ceramic polymer composite with BaTiO3/ PDMS with simple low cost hydrothermal methods by mixing of BaTiO3 with polydimethylsiloxane (PDMS) polymer. The fabrication and extraction of voltage and current from Piezo electric device was interesting, but the output current from the Piezo-composite was found low. The addition of piezoresistive material PEDOT:PSS reduced the output voltage slightly but it improved the output current. So in this scenario, we are interested to study the effect of ZnO, Graphene Oxide on piezoelectric properties of the ceramic polymer composite BaTiO3/ PDMS. Studies of both the effect of composition and temperature on performance will be presented.

Key Words: BaTiO3/ PDMS composite, ZnO, GO, PEDOT:PSS, Piezo energy harvesting

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Abstract ID: 483

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Solar Cells

Keywords: thiophenes, cyclic voltammetry, fluorescence, donor/acceptor, crystal structures

Structural, Electrochemical and Optical Properties of Small Organic Molecules for Solar Cell Applications

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We developed synthetic strategies to design a variety of donor /acceptor molecules based on triphenyl amines, oligothiophenes, oligo etheylenedioxy thiophenes and ladder type fused heterocyclic oligomers endowed with strong acceptor moieties incorporating tricynovinyl-, dicyanovinyl-, halogens, and TCNQ- like groups. The single crystal structural analyses of a wide range of closely related molecules offer insights into the role of various groups in driving the observed packing motifs. Furthermore, we used cyclic voltammetry to characterize the electron donating and accepting abilities of these materials in solution and to provide insights into the evolution of the relative HOMO-LUMO levels as a function of introduction of specific substituents. We also carried out optical characterization of these materials with emphasis on fluorescence and solvatochrmoic behavior as a function of structural modification. By systematically tailoring the molecular structure we monitored how optical and electrical properties evolve. Finally, we use the shifts in CN stretching frequencies in these materials as a possible feature to render them useful as biological markers.

Abstract ID: 485

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Bio-inspired design of composites

Keywords: bio-inspiration, functional composites, sensor

Bio-inspired Composite Fibers as Versatile Sensors

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One of the many challenges in materials science is to minimize the differences between naturally formed structures and manually fabricated morphologies due to the high-performance properties many bio-systems possess while synthetic materials do not have. Specifically for one-dimensional (1D) thin-diameter fibers, the control of their chemical composition and the physical phases is critical in manipulating their mechanical and functional behaviors. Our research relies on tooling engineering of the spinneret that manufactures composite fibers of different polymers and nanoparticles, leading to efficient mechanical enhancement and stimuli-responsive properties. The structure of the composite fibers mimicking the blood vessel with co-axial layers composed of polymer-nanoparticle-polymer channels. A couple of polymers have demonstrated the feasibility of using this unique structure in sensors that responded to mechanical strain (i.e., tension, compression, bending, etc.) and chemicals (i.e., liquid and gaseous volatiles). The high sensitivity to air pressure can go down to 1 psi with high consistency and the selectivity to different solvents could also be proven with low concentrations. The sensing mechanism dependent upon the electrical conductivity has also illustrated the efficiency in controlling morphologies of the nanoparticle channels, including the dispersion quality, continuity, and alignment degrees.

Key Words: bio-inspiration, functional composites, sensor

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Abstract ID: 486

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Processing and manufacturing technologies

Keywords: additive manufacturing, nanoparticles, sensor

Additive Manufacturing of Polymer/Nanoparticle Composites

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Inventions of new manufacturing methods can innovate down-to-nanoscale material structural control and revolutionize the process of large-scale manufacturing, including logistics and green chemistry. The appearance of additive manufacturing, alternatively termed as 3D printing, is well-known to reduce material waste and be more flexible with complex material design. However, the uses of multiple materials in additive manufacturing has so far been limited to a few polymers and continuous carbon or glass fibers. Our research here reports the uses of 3D printing and how it can include non-continuous nanoparticles in the polymer matrix and manage the location and orientation of nanoparticles. The layer-by-layer assembly can be coherently incorporated on the printing platform so that on the delicately-printed surface morphologies, the nanoparticles can be selectively deposited and oriented. The well-controlled nanoparticle topologies showed anisotropic features that maximized the conductivity along specific axis among all directions. We took advantage of the conductive properties for sensing applications and demonstrated the feasibility in using the manufactured structures for chemical sensors, especially volatile organic compound gases. Our project exhibits the newly innovated manufacturing process and how its autonomy improves the processing efficiency of chemi-resistive sensors.

Topic: Processing and manufacturing technologies

Key Words: additive manufacturing, nanoparticles, sensor

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Abstract ID: 487

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Optical properties of metals and non-metals

Keywords: Polymer, Nanostructure, nonlinear properties, absorption, refractive index

Nonlinear optical properties of nanostructured titanium dioxide embedded Poly(methyl methacrylate) using the Z-scan technique

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The nonlinear optical properties of polymers are very important mainly due to their applications in photonic devices. Embedded nano particles in polymers extremely increase surface area because of proportionally more surface atoms than their microscale counterparts, thus allowing intimate interphase interactions and conferring extraordinary properties to the polymer. In this study thin film of Poly(methyl methacrylate)(PMMA) embedded with nanostructured titanium dioxide at various molar concentration was synthesized using casting method.

Nonlinear optical properties, such as nonlinear absorption coefficient, nonlinear reflective index and third-Order nonlinear optical susceptibility of these nanostructured titanium dioxide embedded Poly(methyl methacrylate) thin films using the Z-scan technique were measured. In this measurement CW green laser of 532 nm wavelength and 100 mW power was used in the Z-Scan. The results are useful for application of such polymer in optoelectronics devices.

Abstract ID: 488

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanomaterials and Nanotechnology

Keywords: molecular wire, electron transport, molecular electronics

Molecular Junction Built-in Nanowire Synthesis and Electrical Characterization

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Electron transport through a molecular junction is the most fundamental characteristic for molecular electronic devices. Molecular junctions can be prepared using a prior sophisticated break junction methods, such as mechanically or scanning probe controlled break junctions or electromigration, to create nanometer scale separated metallic contacts and self-assembly of a molecule in the gap. Electrical coupling between the molecule and the contact is another concern when charge transfer of a molecular circuit is considered. A molecular junction built in hybrid nanostructure in a form of metal-molecule-metal however will provide a useful interconnect for molecular electronics enabling a reliable and strong metal-molecule coupling.

This talk will cover synthesis of a novel self-assembled polymeric molecular junction of biphenyl dithiol (BPDT) in the middle of a Au nanowire with a total length of 7.5 - 8.0 micrometer and 300 nm diameter. The extent of the polymeric BPDT molecular section in the hybrid nanowire was made in 20 to 30 nm to study length dependent charge transport through DC mode room temperature I-V measurements. A single hybrid nanowire was trapped across a lithographically defined microelectrode pair using AC dielectrophoresis. The current carrying capacity of the molecular junction were determined in the nano and microamper regimes with interesting I-V characteristics, showing repeatable conductance switching and hysteresis. The first voltage sweep led to a change in the conduction state of the molecular junction from insulating to conducting around 1.4- 1.6 Volt. A sudden increase in the current was characteristics of most of the hybrid nanowires with a few exception of negative differential conductance behavior. Continuing voltage sweep from -4 to 4 V led to nonlinear response with hysteresis once conductive state was achieved for the molecular junction.

This novel nanowire with molecular junction was characterized using SEM and EDS and its electron transport characteristics studied thoroughly to produce repeatable and interpretative I-V measurements.

Abstract ID: 489
Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)
Oral Presentation
Topics: Dielectric materials
Keywords: Dielectrics, aerosol deposition, ceramic capacitor

Development of Ceramic Dielectric Films for Power Inverters in Electric Drive Vehicles

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Future availability of high-temperature power inverters will advance the market share for electric drive vehicles EDVs) that are highly fuel-efficient. An integral part of vehicle power inverters is the DC buss capacitor, which has a significant influence on inverter lifetime, reliability, cost, and temperature of operation. The drive train and backup systems in electric vehicles utilize AC power drawn from a battery via a power inverter. Large ripple currents are produced due to imperfect inversion and rectification. Ripple currents reduce the battery performance, lifetime, and charge/discharge efficiencies. Capacitors are thus used in the power inverters/converters to block ripple currents from reaching the power source. The capacitors currently used in the inverter systems are made of polypropylene films, which lack the ability to handle ripple current at temperatures above 85°C; therefore, dedicated secondary cooling systems are required to provide further cooling of the power electronics in EDVs. Advanced power inverters for EDVs require capacitors that operate at high voltages and high-temperatures at under-hood conditions, and yet have minimal footprint. Argonne is developing lead lanthanum zirconium titanate (PLZT)-based film capacitors for high-temperature power inverter applications. PLZT-based capacitors have the greatest potential for volume reduction; they could be as small as 30% of the volume of a polymer-based capacitor currently used in electric vehicle inverters. PLZT-based capacitors offer high dielectric constants and breakdown fields and, therefore, high energy densities. They can also tolerate high temperatures, enabling them to carry large currents even at elevated temperatures. We have developed a high-rate aerosol deposition (AD) process to produce thick PLZT films with desirable high voltage and high-temperature properties. The AD process is based on collision adhesion of fine ceramic particles with the substrates. The AD process can produce dense films at room temperature without a need for high temperature sintering, thus making the process amenable for depositing PLZT films on a variety of substrates such as polymer, glass, and metal foils. PLZT-based films deposited by the AD process exhibited dielectric constant of ≈80 at 300 V bias, dielectric loss <1%, mean breakdown voltage of ≈1000 V and temperature-dependent properties suitable for advanced power inverters. Recently we fabricated ≈30-cm long and ≈2.5-cm wide PLZT films on aluminum-metallized thin polymer substrates. These PLZT films were wound into capacitors with terminations. The dielectric properties of the PLZT films and the wound capacitors will be presented in this talk.

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Key Words: Dielectrics, aerosol deposition, ceramic capacitor

Abstract ID: 490

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanomaterials and Nanotechnology

Keywords: Thermal Evaporation, Nano-crystalline TiO2, Blue-green emissions

Physical Properties of Nano-crystalline TiO2 thin films prepared by Thermal Evaporation

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We have successfully grown the nano-crystalline TiO2 thin films on BSG substrates by thermal evaporation technique. XRD patterns revealed a mixture of anatase and rutile phases. The origin of the mix phase confirms the source material itself. The FESEM image of the TiO2 films exhibits high-quality nano-crystalline structure with uniformly distributed identical grains of ~22 nm size. The samples show significant transmission in the entire spectrum, which slowly increases from the visible side (45%) to the NIR side (85%). The thickness of the films is approximately 92 nm. The refractive index of the sample displayed a rapid decrease in the UV region, while in the visible and IR regions, it recorded a slow decline. Transmission data also confirmed the nano-crystalline growth of the films. PL spectra exhibited many luminescence peaks, which suggest potential applications and also confirmed the bandgap observations obtained from the transmission spectrum.

Abstract ID: 491

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Hybrid cells for energy harvesting

Keywords: indoor light harvesting, DSSCs, solar cells, copper complexes, IoT

Diffuse Light Harvesting to Structured Information with Dye Sensitized Solar Cells

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By 2025 about 75 billion IoT devices will be installed, of which the majority will reside indoors. It is therefore crucial to find an energy source that yields high efficiencies in this environment.(1,2) At 34% efficiency under ambient light, while being more environmentally friendly, sustainable to produce and to recycle. Dye-sensitized solar cells (3,4) (DSCs) are known for efficient conversion of ambient light. Fast charge separation in a variety of organic dyes and tunable energy levels in CuII/I redox systems combined with negligible recombination processes allow DSCs to maintain a high photovoltage under ambient light. (5,6) The co-sensitization of absorbers enables absorption over a broad spectral range and the adaption to the vast majority of light sources. As a result, DSCs outperform organic photovoltaics as well as silicon and thin-film GaAs technology under ambient lightning.1 We studied DSCs with CuII/I(tmby)2 (tmby = 4,4',6,6'-tetramethyl-2,2'-bipyridine) electrolyte based on a combination of dyes XY1 and L1. The new dye sensitized “solar” cells achieve an unprecedented power output of 103.1 μW cm-2 at 1000 lux.

The harvested “indoor” energy can be used to provide power to all crucial elements of IoT: communicate, sense and process. A major step forward was demonstrated as even machine learning and advanced image recognition is possible on these devices with the given energy for both learning and prediction. There is no need connect to an external power source or save energy (batteries) to prolong their lifetime, our system is designed to use all of the available energy at any given time. Through thorough characterization, we can directly link the number of photons required for a computational inference: 2.72·1015 photons/inference. This is essentially the direct transformation of high entropy diffuse light into structured information.

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Abstract ID: 492
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Design and application of composite structures
Keywords: Functional Composites, 3D Printing, optimization, Engineering Application

Optimum Design and Additive Manufacturing of Composite Materials in Civil Engineering Applications

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In the present study, a composite float design, optimization and additive manufacturing (3D printing) was undertaken based on performance constraints and test setup requirements. For this purpose, commercially available composite materials were taken into account in terms of density, temperature resistance, and alkali resistance, resulting in two design alternatives as Polypropylene (PP) and carbon fiber filaments, as well as resin material. Then the structural configurations were considered and a performance-based design was implemented. In order to minimize the length of the composite float to make it fit well into the test setup, the design problem was formulated into a constrained optimization problem with different design scenarios, and the optimization was conducted using metaheuristic algorithms. The results obtained showed that the solutions of GA and PSO were comparable, however, those of PSO proved to be more accurate in case of more complex design scenario, and also two to three times faster. The manufacturing was conducted through additive manufacturing (3D printing). It was found that the laminated structure of the 3D printed float was pervious, hence resulting in leaking issue. However, the 3D printed float by resin was watertight and suitable for the application in the test setup.

Abstract ID: 493

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: Graphene, Nano, Factorial Analysis, Design of Experiment, LPCVD

Factorial Analysis of LPCVD Graphene Growth

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Quality control of graphene growth is indispensable to graphene-based applications. Most previous studies on graphene growth focus on individual and independent effects of process parameters ranging from CH4/H2 ratio to cooling rate, one factor at a time. In this study, a factorial analysis of graphene quality under different low-pressure chemical vapor deposition (LPCVD) conditions is conducted through a fractional factorial design of experiment method. Five key process parameters are identified in the LPCVD graphene growth process, including the CH4/H2 ratio, growth time, growth pressure, growth temperature, and cooling rate. The graphene quality of as-grown samples is examined with respect to the number of graphene layers based on the I2D/IG ratio response and the number of graphene grains with SEM images. Statistical analysis of the experimental result reveals interaction effects as well as the major and minor effects of each factor. For the I2D/IG ratio response, the major factors are growth time, growth pressure, and growth temperature. The interaction analysis of the I2D/IG ratio response shows that there is a strong interaction effect between growth pressure and growth temperature and between CH4/H2 ratio and cooling rate. For the number of graphene grains, the major factors are growth time and growth pressure. The interaction analysis show that there are strong interaction effects between CH4/H2 ratio and growth time, growth pressure, and growth temperature, respectively. There are also interaction effects between growth time and growth pressure, growth time and cooling rate, and growth temperature and cooling rate. For monolayer graphene growth with larger grain size, the favorable condition is identified as low CH4/H2 ratio, short growth time, high growth pressure, high growth temperature, and slow cooling rate. Although further study is required to understand fundamental mechanisms of the interaction effects, this research provides a guideline to control the quality of graphene via LPCVD growth on the number of graphene layers and graphene grain size.

Abstract ID: 494

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Magnetism and Magnetic Materials

Keywords: Ferromagnetism, ferroelectricity, magnetoelectric effect.

Effect of Co-doping in KNbO3 samples on the multiferroic properties at room temperature

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In this work, polycrystalline KNb1-xCoxO3 (x = 0.00, 0.03, 0.05, 0.07 and 0.10) samples were synthesized through standard solid-state reaction using high- K2CO31.5H2O (98.5%), Nb2O5 (99.95%) and Co3O4 (99.9985%) as starting precursors. The precursors in the appropriate stoichiometric ratio were mixed and grounded in an agate mortar for 2 h; powders were preheated at 150 °C for 2 h, 600 °C for 4 h, 800 °C for 6 h (doped samples) and 900 °C for 6 h (undoped samples), with heating and cooling of 3 °C/min. The powders were then pelletized (5 mm in diameter) using a cylindrical press at a pressure of 3 Ton for 5 min. Afterwards, the pellets were sintered in air atmosphere. The crystal structure of the pellets was analyzed by X-ray diffraction (XRD) in order to corroborate the structure and crystalline phase of the synthesized material. For x = 0.00, 0.03 and 0.05 the diffractograms show no impurity peaks, which evidence that the compounds are single-phase, but for x = 0.07 and 0.10 a secondary phase was found. The recorded X-ray spectra were refined by Rietveld method from which the lattice constants were obtained. Scanning Electron Microscopy and X-ray Energy Dispersion Spectrometry analyzed the morphology and chemical composition, respectively. The electrical properties were studied by means of Electrical Polarization vs Electric Field and Complex Impedance Spectroscopy measurements; ferroelectricity was evidenced for all samples. Magnetization Measures vs Magnetic Field reveals paramagnetic behavior for KNbO3 and the emergence of a weak ferromagnetism in doped samples. In $x \geq 0.05$, they did not improve ferromagnetism and probably the solubility limit of cobalt ions is for $x < 0.05$. Finally, measurements of Electric Polarization vs Electric Field at room temperature were performed with electric fields up to 15 kV/cm, frequency of 100 Hz, and static magnetic field variations of 0.2, 0.4, 0.6 y 0.8 T. The value for the strength of the magnetoelectric coupling obtained is 6.4 % for x = 0.03. . Interactions between bound magnetic polarons are considered as a possible mechanism to explain the appearance of the ferromagnetic signal in the Co-doped samples [1], [2].

Abstract ID: 495

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Bio-composites

Keywords: Polycaprolactone, Bone morphogenic protein, Umbilical cord serum, Osteogenesis

Synergistic effect of alginate/BMP-2/Umbilical cord serum-coated on 3D-printed PCL biocomposite for mastoid obliteration model

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Recombinant human bone morphogenetic protein-2 (rhBMP-2) has been used widely in bone tissue

regeneration; however, the use of rhBMP-2 can be limited clinically because extremely high doses can

cause opposing effects on bone formation, such as high inflammation, edema, and even uncontrollable

bone growth. To overcome the limitation of using BMP-2, we used an umbilical cord serum (UCS) that

exhibits various growth factors (epidermal growth factor, transforming growth factor-β, nerve growth

factor, etc.). To evaluate the effect of the UCS, we studied the synergistic effect of the composite scaffold

using BMP-2/UCS/alginate coated on three-dimensional mesh-structured poly-e-caprolactone (PCL),

both in vitro and in vivo, using a rat mastoid obliteration model. The newly suggested biocomposite

scaffold (BMP-2/UCS/alginate) demonstrates significantly rapid new bone formation (particularly, in the

interstitial area of the scaffold) compared to those of two controls: PCL mesh structure coated with

alginate, and BMP-2/alginate-coated PCL scaffold. Based on the in vitro and in vivo works, the present

study demonstrates that the simultaneous use of low-dose BMP-2 and UCS increases osteogenesis

significantly in a rat model compared to the control that uses only BMP-2.

Abstract ID: 496
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Nanocomposites
Keywords: Polymer-dispersed-liquid-crystal, Clay, Nanocomposite

Polymer-dispersed liquid crystal nanocomposites comprising montmorillonite clay modified by conducting pentamerous oligoaniline

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Pentamerous oligoaniline (POA) was protonated with sulfuric acid to form emeraldine salts (ES) and then intercalated in montmorillonite (MMT) CL120 to develop a functional conductive organo-layered material. The characteristics of the modified clay CL120/ES-POA were analyzed by wide-angle X-ray diffraction (WAXD) to find the d-spacing of the MMT layer distance, and by Fourier transform infrared (FTIR) spectroscopy for the oligoaniline functional group in CL120/ES-POA, and highresolution thermogravimetric analysis (TGA) to determine the theoretical intercalation capacity of the modifying agent in the clay. We successfully intercalated the ES-POA into the MMT by ionic exchange reaction. Polymer-dispersed liquid crystal (PDLC) composites were prepared from the modified clay of 1 wt% loaded in the mixtures of 49 wt% photosensitive monomer and 50 wt% nematic liquid crystal (NLC), in a specific case, so as to generate novel functional nanocomposites. The hybridization of CL120/ES-POA clearly improved the electro-optical properties of the PDLCs. In this work, doping CL120/ES-POA at 1 wt% beneficially lowered the driving voltage by almost 70%, increased the transmission contrast ratio by five times and reduced the response time from 4.6 to 0.7 ms at 25 Vrms at the expense of the viewing-angle properties.

Abstract ID: 497

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Multiferroics, Nanoparticles, Ferromagnetism

Multiferroic properties of Bi0.95Tb0.05FeO3 nanoparticles

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Influence of particle size of Tb-substituted BiFeO3 nanoparticles on the structural, morphological, magnetic and ferroelectric properties has been studied. Sol-gel method was employed for the synthesis and size of the nanoparticles was tailored by variation of calcination temperature (450°C (T4), 650°C (T6)) [1]. X-ray diffraction patterns revealed slight distortion of rhombohedral phase (space group R3c) with Tb-substitution [2]. Peak broadening along with peak shift has been observed with the decrease in particle size, thereby confirming the successful tailoring of particle size [3]. Morphological analysis carried out using Transmission Electron Microscope exhibited high agglomeration owing to the high surface energy of the nanoparticles [1]. Ferromagnetism was displayed by all the synthesized nanoparticles. The observed enhancement of saturation magnetization values with decreasing particle size has been ascribed to surface to volume ratio [3]. Ferroelectric behavior has been found to decay with increasing particle size. Saturated ferroelectric loop with saturation polarization value has been observed for T4. While T5 and T6 exhibited significant change in P-E loop; indicating highly lossy behavior with low values of breakdown voltage [4]. Thus, study indicates enhanced multiferroic properties for smallest particle size thereby, depicting a strong correlation of size and multiferroism.

Abstract ID: 498

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster/Oral Presentation

Topics: Solar Cells

Keywords: DSSC; TiO2; Au; Ions implantation

Improved photovoltaic performance of dye-sensitized solar cells by Au-ion implantation of titania film electrodes

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Plasmonic metal nanoparticles are known to work as light-harvesting antennae and to enhance photocurrents of photovoltaic cells. Therefore, in this work, effect of Gold (Au) ions distribution on the efficiency of dye sensitized solar cells (DSSCs) have been investigated. Thin films of TiO2 have been deposited on FTO glass substrates by doctor tape method. After that Au ions are implanted on these films with different flounce rates (i.e. 2 104, 4 104 and 6 104 ions/cm2). XRD results confirmed that TiO2 is present in anatase phase upto 4 104 ions/cm2 flounce rate. At 6 104 ions/cm2 exposure rate, one peak of rutile is obtained which confirmed that film has mix phases of TiO2. UV results show that dye is adsorbed in all photoanodes. Maximum dye has adsorbed at the flounce rate 4 104 ions/cm2. It is found that the energy conversion efficiency of DSSC is highly dependent of the flounce rate of Au. At the flounce rate 4 104 ions/cm2, cell has high short circuit current density (JSC) i.e. 7.21 mA/cm2, resulting high efficiency ( ) i.e. 2.92%. Impedance spectroscopy shows that the cell which is formed by 4 104 ions/cm2 flounce rate of Au ions has low recombination rate of electron/hole pairs.

Abstract ID: 499
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Multifunctional composites
Keywords: Multiferroics, Nanoparticles, Ferromagnetism

Multiferroic properties of Bi0.95Tb0.05FeO3 nanoparticles

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Influence of particle size of Tb-substituted BiFeO3 nanoparticles on the structural, morphological, magnetic and ferroelectric properties has been studied. Sol-gel method was employed for the synthesis and size of the nanoparticles was tailored by variation of calcination temperature (450°C (T4), 650°C (T6)) [1]. X-ray diffraction patterns revealed slight distortion of rhombohedral phase (space group R3c) with Tb-substitution [2]. Peak broadening along with peak shift has been observed with the decrease in particle size, thereby confirming the successful tailoring of particle size [3]. Morphological analysis carried out using Transmission Electron Microscope exhibited high agglomeration owing to the high surface energy of the nanoparticles [1]. Ferromagnetism was displayed by all the synthesized nanoparticles. The observed enhancement of saturation magnetization values with decreasing particle size has been ascribed to surface to volume ratio [3]. Ferroelectric behavior has been found to decay with increasing particle size. Saturated ferroelectric loop with saturation polarization value has been observed for T4. While T5 and T6 exhibited significant change in P-E loop; indicating highly lossy behavior with low values of breakdown voltage [4]. Thus, study indicates enhanced multiferroic properties for smallest particle size thereby, depicting a strong correlation of size and multiferroism.

Abstract ID: 500
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Composite structural materials
Keywords: Elastic waves, hybrid medium, band structure

Elastic wave propagation in a viscoelastic doped structurally helical solid

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The propagation of elastic waves in helical elastic solid with aleatory distributed nano-spheres constituted by a viscous elastic fluid, is theoretically analyzed. A helical medium isan 1D periodic medium which has an axis of symmetry that revolves around a common helix axis. To take into account the presence of the guest medium (nano-spheres) we usea hybrid medium formalism for calculating the effective stiffness of the composed system. We calculate the band structure of the composite medium and found the appearance of additional band reflections of both handedness near each either of the band edges of the reflection band of the pure elastic helical structure.

Abstract ID: 501

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Multifunctional composites

Keywords: Core-shell nanostructures, piezoresponse, piezoelectric switching, and hysteresis

Ferroelectric effect in ZnFe2O4-BaTiO3 core-shell nanostructures

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Ferromagnetic-ferroelectric (/core-shell) nanostructures are of interest for the single device component with multifunctionality which arises from their strong coupling between ferromagnetic and ferroelectric ordering. Importantly, this type of multifunctional nanostructures will be very useful in various practical applications such as nanoelectronics, magnetic data storage, optoelectronics, and spintronics [1]. We have synthesized ZnFe2O4-BaTiO3 (2:3) core-shell nanoparticles with a diameter of 60 nm from a one-step polyol method. X-ray diffraction and Raman spectra showed the peaks corresponding to tetragonal BaTiO3 (BTO) and cubic ZnFe2O4 (ZFO) phases. Morphology of the core-shell structure of the calcined NPs at 650 oC is studied using Scanning Electron Microscopy (SEM) and Scanning Probe Microscopy. We found that the BTO shell material grown over the ZFO core due to the lattice mismatch between the ZFO and BTO as ZFO has a large strain value (0.008) with the reduced tetragonality (c/a = 0.991). Study of ferroelectric polarization and its domain structure of the ZFO-BTO core-shell NPs are conducted by piezoresponse force microscopy (PFM) in the voltage range from -7 to +7 V with a step of 1 V. The local piezoelectric switching is observed in the BTO shell region at dc bias of ± 7 V. This study also revealed that the core-shell nanostructures are having less ferroelectric polarization in comparison to that of BTO. This is attributed to the encapsulation of the ZFO core within the BTO shell material.

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Abstract ID: 502

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: nanocrystals, nitroarene reduction, pseudomorphic conversion, rhombic dodecahedra, silver oxide

Formation of Silver Rhombic Dodecahedra, Octahedra, and Cubes through Pseudomorphic Conversion of Ag2O Crystals with Nitroarene Reduction Activity

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Using ethanol as a co-solvent, relatively small-sized Ag2O octahedra (~645 nm in opposite corner distance), and rhombic dodecahedra (~540 and 655 nm in opposite face distance) were synthesized in aqueous solutions. Ag2O cubes synthesized in an aqueous solution have an edge length of ~425 nm. Band gaps of these crystals have been obtained, revealing presence of facet-dependent light absorption properties. The Ag2O rhombic dodecahedra, octahedra, and cubes were treated with ammonia borane in ethanol at 50 ºC for just 10 min to pseudomorphically convert to Ag polyhedra of the corresponding morphologies. Transmission electron microscopy (TEM) characterization confirms the Ag cubes, octahedra, and rhombic dodecahedra are bound by the {100}, {111}, and {110} faces, respectively. The Ag rhombic dodecahedra, available for the first time, showed more superior catalytic activity toward 4-nitroaniline reduction at 50 ºC than Ag octahedra and cubes, and gave 100% product yield after 1 h of reaction. This work demonstrates the value of forming Ag rhombic dodecahedra exposing {110} surfaces that may be useful in other organic transformations.

Abstract ID: 503

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: Tellurene, Thermal Annealing Technique, 2D Thickness Control, Raman spectroscopy

Thickness Control of Exfoliated Tellurene: Towards Obtaining Few Layers Tellurene

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Tellurene (Te) has become the focus in 2D materials due to its tunable bandgap, anisotropic behavior, and resilience to the ambient conditions.[1] Nonetheless, Te flake exfoliation is challenging and suffers from low yield due to its crystal structure and layer to layer bonding. Consequently, fabrication of a few layers Te is limited to epitaxial growth or liquid exfoliation.[2,3] In this work, we report a thermal annealing technique conducted in a controlled oxygen environment applied to mechanically exfoliated Tellurene. According to our AFM measurements, a significant decrease in thickness is observed for Te nanosheets from bulk (~1µm) to few layers (~25nm). This thinning has been confirmed using Raman spectroscopy, where a clear blue shift measured for A1 and E2 Raman modes after thermal annealing. We observe a favorable thinning direction for all thinned Te nanosheets, which is attributed to the anisotropy behavior of these Te nanosheets. Our results shed some light on a simple annealing technique for future Te device applications.

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Abstract ID: 505

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multiscale Modeling in Mechanics and Composite Materials

Keywords: Nanocomposites, CNT, Micromechanics, Dynamic analysis

Dynamic Analysis of CNT Reinforced Nanocomposites using Nonlocal Micromechanics Homogenization and Thickness Stretching Models

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Estimation of effective material properties of carbon nanotube (CNT) reinforced nanocomposites, is one of the important challenges in studying the mechanical response of these structures. A novel nonlocal formulation is adopted to develop the representative volume element (RVE) of the well-dispersed CNT fibre in polymeric matrix. The finite element approach is used to solve the governing system. This approach tries to do away with the conventional practice of representing efficiency parameters to scale the size effects in extended rule of mixture based continuum approach. Further, we present an elasticity based RVE model to verify the results with simple rule of mixture based homogenization. A cylindrical RVE is selected and subjected to the conditions of pure tension, internal lateral pressure and pure twisting to specify the effective material properties. The effective material properties are utilized to study the dynamic response of CNT reinforced sandwich panels. The free vibration as well as transient dynamic analysis is performed. The highly heterogeneous nature of nanocomposites demands the refined kinematic models to study the mechanical response. This study considers a shear and normal deformable theory without the necessity of including shear correction factor. This model is well tested for functionally graded (FG) composites. The model is versatile to consider the membrane and bending behavior of shell structures which could be highly complex at times. A finite element scheme with eight node isoparametric element is considered and effect of volume fraction of CNTs on the vibration response of the nanocomposites is studied. Through an optimized distribution of the CNTs, the dynamic response could be tailored for the desirable functions of these structures. The consideration of CNT agglomeration at the level of RVE modeling and manufacturing limitations of CNT profiles still pose interesting challenges for future research.

Abstract ID: 506

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: Atomic Catalyst; Graphdyine; Mapping;

Mapping of atomic catalyst on graphdiyne

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Atomic catalysts (AC) as the frontier in atomic catalyst have attracted tremendous attention in recent electrocatalyst research [1]. The performance of ACs strongly depends on the electronic interaction between the atoms and support. To supply a direct strategy for discovering more promising electrocatalysts, we propose a comprehensive mapping study of anchoring transition metals on the graphdiyne (GDY) [2]. The electron transfer ability and zero-valence stability are quantified based on the redox process between surface metal and GDY support. The different electron transfer number and directions between the transition metals and GDY are also compared, in which the initial one-electron transfer is the most difficult. Among all the TMs, Co, Pd and Pt have displayed the exceptional stability of zero-valence catalyst based on the evident energy barrier difference between losing electrons and gaining electrons. Experimental results support the remarkable performance of our screened candidates, which have opened a new possibility to achieve novel high-performance zero-valence ACs. Moreover, we outlook the introduction of the deep-learning algorithm in the future advanced mapping strategy for achieving more complicated ACs [3]. This work not only supplies innovative electrocatalyst candidates but also exhibits an innovative approach for studying the electrocatalysts that can further apply to more material systems.

Abstract ID: 507
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Polymeric composites
Keywords: liquid silicone rubber (LSR), HVDC breakdown strength, silicone rubber nanocomposite

Effect of Nanosilica-modification on HVDC Breakdown Strength and Tensile Property in Silicone Rubber Nanocomposites

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Hydrophilic surface of a nanosilica is changed to hydrophobic characteristics by modifying with various ratio of alkylsilane and vinylsilane coupling agents. The effects of the modified nanosilicas on high voltage direct current (HVDC) breakdown voltage and tensile property in silicone rubber nanocomposites are studied in order to apply them to heavy electric equipments. The surface modification is confirmed by Fourier-transform infrared spectroscopy (FT-IR) analysis and the weight of the alkyl/vinyl coupling agents is measured by thermogravimetric analysis (TGA). Silicone rubber nanocomposites are prepared by mixing a liquid silicone rubber (LSR) and the modified nanosilicas. The mixing ratio of LSR to the nanosilica is fixed to be 20 wt%. To observe the even dispersion of nanosilica particles in the LSR matrix, transmission electron microscope (TEM) is used and it is found that the surface-modified nanosilicas are well dispersed in the form of nano-clusters with 20-100 nm size. Electrical properties (±HVDC breakdown strength and dielectric properties) and mechanical properties (tensile strength and elongation-at-break) are estimated, and ±HVDC breakdown strength and tensile strength are maximum when the surface modification ratio of alkyl silane : vinyl silane is 50 : 50 wt%. Dielectric permittivity increases slightly with the alkyl/vinyl ratio owing to the unreacted vinyl group.

Abstract ID: 509

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: cellulose, nanocomposites, silver-zinc oxide, ecotoxicology, characterization

Biomediated cellulose-Ag-ZnO nanocomposites and their ecotoxicological assessment using onion bulb plant

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The incorporation of nanoparticles into cellulose materials to form a nanocomposite is an interesting way of improving the functions and applications of the cellulose [1,2]. The properties associated with the nanoparticles contribute immensely to the overall behavior of the nanocomposites, which determines their applications. Biosynthesis of nanoparticles is an ecofriendly method of synthesis and some metals such as Zn and Ag have been used in biological systems over the years. Cellulose-Ag-ZnO nanocomposites has been prepared using litchi peel extract and characterized by UV-visible and FTIR spectroscopic techniques, powdered X-ray diffraction (XRD) and transmission electron microscopy (TEM) analysis. The characterization techniques revealed the structure of the nanocomposites, which is composed of cellulose, Ag and ZnO, and the nanoparticles were agglomerated within the matrices of the cellulosic material. An ecotoxicological assessment of the nanocomposites was carried out using onion bulb plant to scientifically ascertain the benign nature of the biosynthesized materials. The results showed that exposure of the plant to increased concentration of the nanomaterials resulted in toxicity, which indicated that the nanocomposites are slightly toxic to the onions plant.

Keywords: cellulose, nanocomposites, silver-zinc oxide, ecotoxicology,characterisation.

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Abstract ID: 510

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Electrochemical Supercapacitors

Keywords: Washnut, Nanoporous Carbon, Chemical Activation, Energy Storage

Nanoporous Carbon Materials Derived from Washnut Seed with Enhanced Electrochemical Supercapacitanc

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Hierarchical nanoporous carbon materials with high surface area, well-developed porosity, interconnected meso- and micropore structure and high conductivity offer wide range of technological applications including sensing, separation, purification and energy storage.1 Here we present a new nanoporous carbon materials derived from the agricultural waste, Washnut seed by zinc chloride chemical activation method.2 Pre-carbonized (300 °C in air) Washnut seed powder was mixed with zinc chloride (1:1 wt ratio) and carbonized at different temperatures (400 to 1000 °C) under a constant flow of nitrogen gas (120 cc/min). The prepared carbon materials contain both micro- and mesoporous architecture as confirmed by nitrogen sorption measurements. All the samples display type-IV sorption isotherm. BET surface area and total pore volume of the optimal sample (carbonized at 800 °C) ca. 865 m2/g and 0.414 cc/g, respectively. Electrochemical (cyclic voltammetry and galvanostatic charge-discharge) measurements in a three-electrode system in an aqueous electrolyte (1 M H2SO4) revealed that the Washnut derived nanoporous carbon materials show excellent supercapacitance performance. Specific capacitance of optimal sample is ca. 162 F g–1 at a scan rate of 5 mV s–1 and 205 F g–1 at a current density of 1 A g–1. Due to the hierarchical bimodal pore architecture containing both meso and micropores, the electrode showed high rate capability sustaining 71% specific capacitance at high current density of 20 A g–1 demonstrating the potential of the materials in high rate performance supercapacitor electrode design. This study showed that nanoporous carbon materials from agricultural waste using a simple chemical activation method can be used for development of high-performance electrode materials for electrochemical supercapacitors.

Abstract ID: 511

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Design and application of composite structures

Keywords: Microbial Synthesis, Pd Alloy, Graphene, Electrochemical, Atomic level

Microbial Synthesis of Pd Alloy for Highly Superior Electrochemical and Electrocatalysis Performance

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Structure-engineered Pd-based catalysts at the atomic level can efficiently enhance the catalytic presentation for oxygen and/or small organic molecules electrocatalysis, equivalent to or even greater to that of commercial Pt/C. Herein, PdCuCo anisotropic structure (AS) electrocatalysts were synthesized with abundant vacancy defects on the exterior surface, which was verified by aberration-corrected transmission electron microscopy and an elemental mapping characterization for the three individual elements were performed as illustrated in Fig.1A. On the other hand, biosynthesis founded on the reducing ability of electrochemically active bacteria is commonly utilized in the reduction of metal ions into nanoparticles as an eco-friendly approach to recover metal supplies. Nevertheless, those bio-nanoparticles cannot be applied precisely as electrocatalysts owing to the weak conductivity of cell substrates. We cracked this problem by a hydrothermal reaction as presented in Fig.1B, which additionally provided a heteroatom doping and alloying between Pd and Au. The aggregation of nanoparticles was prevented with the protection of graphene, and the porous structure was retained, resulting in better durability and electrocatalytic activity than commercial Pd/C under both alkaline and acidic circumstances. The created strategy in this research initiates a prospect into constructing electrocatalysts via entirely utilizing the abundant resources in nature.

Abstract ID: 512

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Graphene, Mxenes and other two-dimensional materials for energy applications

Keywords: Holey graphene, Supercapacitor, Batteries, Water Desalination, Gas sensors, Electrocatalyst, Bioseparation, Fuel cells, Applications

Holey graphene: An Emerging Versatile Material

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Holey graphene, also known as perforated graphene is formed by generating in-plane holes in basal planes of graphene based materials. By exploiting the combined advantages of holes and graphene, the holey graphene based materials have garnered significant interest due to their exceptional properties such as higher electrical conductivity and higher surface area. These remarkable properties have enabled holey graphene based materials to outperform its pristine form (graphene) and demonstrate its applicability in versatile fields including electrical energy storage (supercapacitors, Li-ion, Li-air, Li-S and Na-ion batteries), energy conversion (electro-watersplitting, dye-sensitized solar cells), water desalination, bioseparation, fuel cells, gas sensors, hydrogen storage and dye degradation systems. As a consequence, it is important to uncover the prime properties and the related potential industrial implications of holey graphene based materials for the development of further research. Hence, in the review, the properties of emerging holey graphene-based materials and various applications including principles, design, fabrication, and engineering aspects are discussed in detail. The recent advances in the state-of-the-art hole generation methods in graphene-based materials along with its working mechanisms, associated issues/solutions, and possible future are discussed. Additionally, the review is aimed to provide critical views on the current status, prospects and generate novel ideas for the development of holey graphene-based materials as a formidable candidate for versatile applications.

Key Words: Holey graphene, Supercapacitor, Batteries, Water Desalination, Gas sensors, Electrocatalyst, Bioseparation, Fuel cells, Applications

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Abstract ID: 513

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Nanostructured materials for advanced batteries

Keywords: Lithium-ion batteries, Conversion-type cathodes, Iron(II) fluoride, carbon materials, nanocomposites

Effects of carbon structure and functionalization on the electrochemical performance of FeF2-C composites as cathodes for Li ion batteries

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Fluoride-based cathodes offer an outstanding technological potential Lithium-ion batteries due to their very high volumetric capacities approaching ~ 2000 mAh/cm3 and low cost. The achieved progress in both the fundamental understanding of the Li insertion/extraction from metal fluorides and their performance stability has been quite promising1-2. However, additional experimental effort and diversification of the cathode formation approaches are highly needed in order to approach the commercialization. The effects of carbon structure and functionalization on the performance of iron(II) fluoride-carbon composites was investigated. The synthesis of FeF2 was performed by microwave-assisted conversion of iron metal (Fe) by hexafluorosilicic acid (H2SiF6) to FeSiF6, then a heart treatment of FeSiF6 salt under Argon atmosphere to form FeF2 and release of SiF4 gas1. Such an approach was chosen based on the hypothesis that multiple metals may be uniformly dispersed in precipitated salt precursors and thus in the ultimate metal fluorides2. Furthermore, such a method enables the construction of FeF2-C composite electrodes, whereby the C scaffold provides electrical conductivity and structural support and metal fluoride crystals are controlled to small dimensions. Such studies was motivated by a hypothesis that carbon additives may help to electrochemically connect metal fluoride nanoparticles to the carbon matrix and additionally reduce undesirable electrochemical interactions between FeF2 (or Fe in the discharged state) and liquid electrolytes. In order to synthesize FeF2-C composites, different carbon materials including multiwalled carbon nanotubes, graphene, graphene functionalized COOH, graphene functionalized OH were immersed in the FeSiF6 aqueous solutions overnight to promote thorough wetting of the carbon materials, then the mixture was dried in vacuum oven at 80 ◦C. The FeSiF6-C composites were heat treated at 250 °C for 360 minutes to convert FeSiF6 to FeF2. The desired reactions were confirmed using thermogravimetric analysis and powder X-ray diffraction. In this work, we demonstrated that the general approach of using FeSiF6 precursor can be successfully applied to synthesize different FeF2-C composites. The electrochemical behavior different of FeF2-C composites was studied via galvanostatic charge-discharge experiments (GCD), cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). All electrochemical testing was conducted with Li metal counter electrodes in coin cells. Working electrodes consisted of 1:1 FeF2:C ratio by mass along with a standard PVDF binder, cast onto Al foil. Capacities measured in the first 100 cycles range between 400 and 500 mAh/g. These are all significantly higher capacities than those of commercial intercalation cathodes, which typically exhibit a maximum capacity of ~200 mAh/g or less. It seems that in all cases the carbon matrix helps preserve the morphology, prevent segregation of phases.

Abstract ID: 514

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Production and characterization of composite materials

Keywords: Zirconium; Nitrides; Plasma processing and deposition; Glow discharge; Surface Hardening

Effect of Nitrogen Gas Ratio and Processing Time on the Properties of Pulsed DC Plasma Nitrided Zirconium

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In the present research, the effect of Nitrogen concentrations (60-90%) in Nitrogen-Argon (N2-Ar) gas admixture plasma and processing time (4, 6, 8, and 12 hours) studies during nitriding of zirconium using 100 Hz pulsed DC Plasma system. X-Ray Diffraction results show the presence of non-stoichiometric Zr3N4 and Zr2N phases with different orientations in the nitride layer. However, the insulating/metastable Zr3N4 phase is dominant in the nitride layer, which indicates the presence of higher nitrogen concentration. The texture coefficient, crystallite size, and residual stresses of the nitride layer vary with the varying concentrations of N2 and the processing time. Surface morphology from optical and scanning electron microscopy indicate the creation of a dense and compact zirconium nitride layer. Electrical resistivity measured by the four-point probe method shows the high value (836 Ω-cm) endorsing the presence of insulating the Zr3N4 phase at higher concentrations. Micro-hardness results show a variation in surface hardness with the variation in the concentration Nitrogen as well as processing time due to the increase of density of the nitride layer. The value of hardness is found nine times higher than that of the untreated surface for the sample nitrided in N2-Ar admixture plasma with a concentration of 70% N2 for the time duration of 12 h. The higher surface hardness is attributed to the denser microstructure and texture coefficient in the nitride layer.

Abstract ID: 515

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Optical properties of metals and non-metals

Keywords: lanthanide, hydroxyquinoline, DFT, photophysical, tripodal

Computational and experimental studies on bonding and photophysics of a triaza-macrocycle tripdodal chelator and its lanthanide complexes

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Lanthanides are often used in modern technologies due to their outstanding photophysical, electronic structures, optical and magnetic properties, have encouraged their use in in magnetic resonance imaging (MRI), biological assays, light emitting diodes (LED), telecommunications, optical fibers, light amplifiers, and lasers, etc.. 8-Hydroxyquinoline (HQ) forms luminescent complexes with a large variety of metal ions, which has resulted in their extensive applications in OLED and displayed technology. Anchoring more than one unit of 8HQ enhances the stability, coordination and the optical properties. Hence, a newly developed multifunctional tripodal chelator containing a 12N3 and three HQ units linked through methylene group, viz., 1, 5, 9-tris(-5-methylene)-1, 5, 9- triazadodecane, [12N3Me5Ox], and its three lanthanide complexes (Lu, La and Gd) are described through synthesis, characterization and theoretical technique. For this, the ligand and its three neutral complexes are synthesized and characterized using CHN analysis, FT-IR, molar conductance, 1 H- 13 C NMR, thermogaravimetric analysis and ESI-mass spectrometry techniques. Each Ln3+ complex is eight-coordinate and bonded to three sets of O, N-donors of HQ units and two water resulting in a pseudo-C3 symmetric distorted dodecahedron geometry. In-silico studies by density functional theory(DFT) method suggest that the lanthanide ion can be easily encapsulated in the ligand cavity without changing its basic geometry. The nature of the bonding between the Ln3+ ions and 12N3Me5Ox3-, interpreted through NBO (natural bonding orbital), EDA (energy decomposition analysis), suggests that the metal-ligand bonds have more ~30% covalent character. The covalent nature of the complexes increases in the order Lu > La > Gd. Interesting and diverse behavior has been observed when the results of 12N3Me5Ox were compared with the previous reported 9N3Me5Ox [1,4,7-tris-(5-methylene)-1,4,7-triazacyclonone chelators. The results show that with increase the size of the macrocyclic ring, the covalence of the metal-ligand bond increases. The luminescence spectral studies of the lanthanide complexes were observed in the solid and solution state. No f-f transitions were observed. The experimental finding (vibrational, NMR, excitation and emission behaviour of the ligand and the complexes were explained with the help of DFT and showed good agreement with the theoretical results. Plausible applications of the complexes are also projected.

Abstract ID: 516

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Optical properties of metals and non-metals

Keywords: Hydroxypyranone, electronic spectra, sensor, DFT, fluorescence

Development of Potential Hexadentate Ligand with Hydroxypyranone Scaffold: Studies of Coordination and Photophysical Properties

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Hydroxypyridinonate (HOPO) chromophore, a bidentate ligand is known to sensitize Ln(III) ions. Optimizing lanthanide luminescence entails delicate molecular design to fulfil vivacious elements during the sensitization process. Multiple hydroxypyridinone scaffold in one unit theatrically improve the luminescence properties of the Eu(III) complexes. The unique luminescence properties of such complexes are widely considered as potential substitutes of organic chromophores particularly in biological applications in which autofluorescence from biological entities frequently interferes with fluorescent signals. Kojic acid (KA), 5-hydroxy-2-(hydroxy-methyl)-4H-pyran-4-one, a naturally occurring fungal metabolite, has a bidentate unit is analogues to hydroxypyridinones. It is used as a skin-whitening and anti-browning agent owing to its potent tyrosinase inhibition activity. Its efficacy is reduced due to change in pH, thermal- and photodegradation. To overcome this limitation, many derivatives have been synthesized by the modification of C-2 hydroxyl group. Edifice of a single molecule with KA scaffold can improve the efficacy, chelating properties and medicinal values. Hence, a kojic acid based tripodal scaffold, tris[(5-hydroxy-4-oxo-pyran-2-yl)methyl]benzene-1,3,5-tricarboxylate has been designed, synthesized and characterized by various spectroscopic techniques like UV-vis, IR, 1HNMR, 13CNMR and mass spectrometry. The ligand contains benzene as the central unit, ester group as spacer and kojic acid derivative as the binding moieties with O donors. The acid-base behaviour and coordination properties of the tripodal ligand are investigated with the trivalent metal ions viz., Fe(III), Cr(III) and Al(III) by potentiometric and spectrophotometric methods in a highly aqueous medium (9:1 :: water:dmso). The protonation constants of the ligand and stability constant of its metal complexes were evaluated. At lower pH(~2.5), the predominant species is LH6 due to protonation at the O atom of ester groups, and with the increase of pH, formation of LH3 and LH2 species occurred. At the higher pH, LH species is predominant which could be due to intermolecular H bonding as a result of π−stacking as observed in theoretical studies, which restricts deprotonation of LH species. The thermodynamic properties and structural prediction of the ligand are explored by the theoretical studies using DFT method. The unique geometry of the ligand forces both the kojyl rings to undergo a face to face π−π stacking, while the third ring forms a T-shaped orientation. The fluorescence study of the ligand was carried out in highly aqueous medium at excitation wavelength 260nm, where it exhibits emission at 428.7 nm wavelength. The fluorescence properties were also explored in the presence of a series of biological important metal ions. Enhancement in the fluorescence intensity was observed in case of Ni+2 and Zn+2 whereas, Fe+3 and Cr+3 ions caused quenching of the emission.

Abstract ID: 517

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Production and characterization of composite materials

Keywords: Chitosan fiber, Antibacterial property, Electrical properties, Degree of deacetylation

Study on the relationship between the degree of deacetylation and electrical and antibacterial properties of chitosan fiber and its composite yarn

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Study on the relationship between the degree of deacetylation and electrical and antibacterial properties of chitosan fiber and its composite yarn

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Functionalization of textiles by using environment-friendly materials and green manufacturing technology has been considered as a major direction of development of textile products. Chitosan fiber is a totally degradable and renewable fiber. Due to its attractive inherently antibacterial and antimicrobial properties, safety, unique characteristics for biomedical uses as well as excellent direct skin contact performance such as high level of comfort, the antiallergicity and the high humidity absorption, the applications of chitosan fiber have been extended from medical area to many other areas including textiles. However, the relationship between the degree of deacetylation and the resultant electrical and antibacterial properties is not clear, which results in the large variation of the property of chitosan fibers and the resultant fabrics, including the antibacterial and antiallergic properties. In this study, the degree of deacetylation of chitosan fiber was examined by using colloidal titration method while the electrical and antibacterial properties of fiber were evaluated following GB/T 12703.03 and AATCC 100, respectively. The fiber surface structure and cross-section, fiber length and diameter, and tensile strength and elongation were also tested according to relevant standards. Based on these results, the relationships between the degree of deacetylation and electrical and antibacterial properties of chitosan fiber can be established, and on that basis, the antibacterial mechanism of chitosan fiber can be understood. These relationships are very useful for the setup of specifications of chitosan fiber for achieving the desired antibacterial properties of the fiber and the resultant composite yarn and fabric.

Key Words: Chitosan fiber, Antibacterial property, Electrical properties, Degree of deacetylation

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Abstract ID: 518

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Carbon and metal oxide based composite materials

Keywords: Metal oxides, Activated carbon, Tyres, Nanofibers, Wastewater

Fe3O4-SiO2 coated tyre-based activated carbon nanofibers as a nanoadsorbent for ultrasound assisted dispersive solid phase extraction of arsenic, cadmium and thallium in environmental samples

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The toxicity of trace metals such as arsenic, cadmium and thallium have been well documented and their adverse effects includes sleeping disabilities, speech disorder, high blood pressure, poor concentration, memory loss, mood swings, fatigue, allergic reactions and depression [1]. In addition, arsenic, cadmium and thallium have the potential to disrupt the human cellular enzymes [2]. Therefore, in order to solve the problem that is associated with toxic elements, green and effective sample preparation techniques need to be developed. Therefore, in this study, magnetic iron oxide-silica nanoparticles coated tyre based activated carbon nanofiber (Fe3O4-SiO2@ACNF) nanocomposite was prepared and reported for the first time as a nanoadsorbent for the ultrasound assisted dispersive solid phase extraction (UA-DSPE) of arsenic, cadmium and thallium from complex matrices. The concentrations of As, Cd and Tl were determined by inductively coupled plasma optical emission spectrometry (ICP-OES). The synthesized nanocomposite was characterized by Fourier transform infrared spectroscopy, x-ray diffraction, scanning electron microscopy, transmission electron microscope and Brunauer, Emmett and Teller surface area. Various parameters such as pH, eluent concentration, extraction time and mass of adsorbent were optimized using the response surface methodology based Box-Behnken design. Under optimum conditions, limit of detection (LOD) and quantification (LOQ) of UA-DSPE were 10, 80, 90 ng L-1 and 33, 266, 300 ng L-1 for As, Cd and Tl, respectively. In terms of precision, the relative standard deviation (%RSD) ranged from 0.6-0.8%. Furthermore, the accuracy of the proposed method was verified by spike recovery test and satisfactory recoveries (95-99%) were obtained. Finally, the UA-DSPE method was successfully applied to wastewater (influent and effluent) and river water samples for the extraction and preconcentration of As, Cd and Tl.

Abstract ID: 519

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: Chalcopyrite, WIEN2k, GGA approximation

Ab Initio Study of Electronic Structures of Chalcopyrite for Photovoltaic Application

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The chalcopyrite materials such as CuInSe2 and CuGaSe2 play a very significant role in the development of photovoltaic cells as their band gaps lie in visible region of spectra and hence can prove to be a good absorber in thin film solar cells. Investigations have been carried out to study the electronic structures of CuInSe2 and CuGaSe2 using ab initio calculation with the help of full potential linearized augmented plane wave method (FPLAW) by employing WIEN2k computational package. Calculations have been done using the GGA approximation in the form of Perdew-Berke-Erzndof (PBE) functional to estimate the values of energy gap for both the compounds. The results were found to improve using the PBE plus mBj functional. The values of energy gap for CuInSe2 and CuGaSe2 have been calculated to be approximately 1eV and 1.07eV respectively. The density of states has also been plotted for both the compounds. The obtained results have been found to be in good agreement with the available data in literature.

Abstract ID: 520

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Combined pollution, Visible photocatalysts, Organophosphate flame retardants

Preparation of bismuth series visible light catalyst and its mechanism for removing Cr(VI) and organophosphorus flame retardants

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Organophosphate flame retardants (OPFRs) are characterized by stable structure and good flame retardancy, and gradually replace bromine and chlorine flame retardants in electronic products. In our research, OPFRs and Cr(VI) combined pollution as the research object to prepare high efficiency and low toxicity type visible photocatalysts. The environmental factors influencing the degradation and Cr(VI) reduction of organophosphorus flame retardants under photocatalysis were investigated. The degradation pathway and Cr(VI) reduction mechanism of organic pollutants in the combined pollution system were clarified. Explore the collaborative removal mechanism of pollutants in the combined pollution system with illumination. It provides theoretical basis and technical support for the treatment of compound pollution of organic matter and heavy metal in water environment.

Abstract ID: 521

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Rare Earth-Based Hard Magnetic Materials

Keywords: Electrochemical synthesis, electroreduction, magnetic materials, rare-earth metals, ionic melts

Electrochemical synthesis of magnetic materials based on rare-earth metals in ionic melts

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Electrochemical synthesis of magnetic materials based on rare-earth metals in ionic melts

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Intermetallic and refractory compounds of rare-earth metals with metals of the iron triad and boron have high magnetic characteristics. After the discovery of the unique magnetic properties of alloys such as SmCo5, SmPrCo5, Nd2Fe14B in the early 80s of the twentieth century, the demand for rare-earth metals and their compounds has increased sharply and continues to grow up to now [1]. The main way to obtain magnetically hard materials based on rare-earth metals is the melting of components at high temperatures, followed by dispersion in an inert atmosphere. These processes are complex and occur at high temperatures. In our opinion, one of the most promising methods of preparation may be electrochemical synthesis from molten halides. The basis of the electrochemical synthesis of intermetallic (with metals of the triad of iron) and refractory compounds (borides, silicides) of rare-earth metals we have put together the processes of joint electroreduction of ions of rare-earth metals and metals of the triad of iron (iron, cobalt, nickel), as well as boron (silicon) in chloride melts alkali metals and their subsequent interaction at the cathode at the atomic level with the formation of micro-, submicro- and nanoscale powders of the phases of intermetallic and borides of rare-earth metals. We have studied the processes of electrochemical reduction of lanthanum, gadolinium, neodymium, praseodymium, cerium, samarium, dysprosium, holmium ions in alkali metal chloride melts. The regularities of the processes of the joint electroreduction of the ignogous of rare-earth metals by fluoroborate, fluorosilicate ions and iron, nickel and cobalt ions in chloride melts at 973 K have been established. The electrochemical synthesis of micro-, submicro- and nanoscale iron powders, double borides of rare-earth metals with cobalt and iron has been implemented. The optimal parameters of the electrochemical synthesis of micro-, submicro- and nanoscale powders of borides, silicides, double borides, intermetallides of rare-earth metals and metals of the iron triad are determined: melt composition, electrolysis potential, cathodic current density, electrolysis duration.

Key Words: Electrochemical synthesis, electroreduction, magnetic materials, rare-earth metals, ionic melts.

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Abstract ID: 522

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Epitaxial Materials and Devices

Keywords: MESFET, Thin Film, ZnO, RF sputtering

Fabrication and Characterization of ZnO Based Metal -Semiconductor Field Effect Transistor

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ZnO-based metal-semiconductor field-effect transistors(MESFET) have attracted significant attention in recent years. In the present work, ZnO MESFET fabricated on SiO2/p-type silicon substrate. A 200 nm oxide layer was first grown on a p-type silicon substrate using a thermal oxidation method. On oxide layer 20 nm – 100 nm ZnO thin film deposited using the radio frequency sputtering technique. The ZnO thin film was heat-treated, and deposition was done at elevated temperatures to improve its optical, electrical, structural, and chemical characteristics. The electrical resistivity of the film was probed by four-probe measurements. The film's thickness was measured by an ellipsometer and monitored at the time of deposition. Source/drain and gate deposited on the thin film by photolithography and thermal evaporation method. Electrical characteristics of the metal field-effect transistor were measured with a semiconductor parameter analyzer. The thickness of the film affected the magnitude of the current that flows between source and drain and ON and OFF voltage. Barrier height between the gate and channel was affected by the thickness of the film. The depletion width formed between the semiconductor and metal gate depends on the thickness and decides the current magnitude. It is found that the p-type of the substrate produces opposite electrical characteristics than as expected in the case of MESFET. In general in MESFET Schottky contact formed between the semiconductor and metal gate. Due to Schottky contact, a depletion width forms at the interface of the semiconductor and metal gate. Gate and semiconductor junction can be forward and reverse biased on applying positive voltage and negative voltage at the gate. Positive bias at the gate reduces the potential barrier, and in turn, the current magnitude between the source and drain increases. However, the reverse was obtained for the negative potential application at the gate because we have used p-type substrate.

Abstract ID: 523
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Multifunctional composites
Keywords: Mechanical Metamaterial; Multifunctional composite; Energy harvesting; Additive manufacturing.

Multifunctional Composite Mechanical Metamaterials for Sensing and Energy Harvesting

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Mechanical metamaterials gain their tailored unprecedented/counterintuitive mechanical properties from their rationally-designed structures rather than inheriting them directly from their chemical composition. A substantial portion of the current effort in the arena of mechanical metamaterials has been merely going into exploring new geometrical design of micro/nano-architectures to improve or identify unusual sets of mechanical properties. Arguably, there is a critical shortage in research needed to engineer new aspects of intelligence into the texture of mechanical metamaterials for multifunctional applications. This study aims to create a new generation of multifunctional composite mechanical metamaterials called self-aware composite mechanical metamaterial (SCMM) with complex internal structures toward achieving self-sensing and self-powering functionalities. We develop finely tailored and seamlessly integrated microstructures composed of topologically different materials to form a hybrid mechanical metamaterial system. Since an SCMM is composed of different materials that are organized in a periodic manner, it will also offer boost the mechanical properties such as enhanced strength and stiffness. Theoretical and experimental studies are conducted to understand the mechanical and electrical behavior of the multifunctional SCMM systems. Furthermore, we highlight the application of the proposed SCMM concept by prototyping self-sensing shock absorbers with energy harvesting capabilities.

Abstract ID: 524

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Magnetism and Magnetic Materials

Keywords: Mossbauer-Spectroscopy, Hyperfine Interactions, Magnetic characterization

Revisiting Mossbauer-Spectroscopy Characterization of Magnetic Materials

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There are three kinds of hyperfine interactions observed in a Mossbauer spectrum. Mossbauer spectroscopy gives quantitative information on the isomer shift (δ), electric quadrupole splitting (Δ or QS), the magnetic hyperfine field (MHF), and Curie or Neel temperature (TC or TN) of iron-based magnetic materials. The δ (Coulomb interaction between protons of the nucleus and s electrons) is related to iron oxidation state, spin state and bonding properties, the Δ (interaction between the nuclear quadrupole moment of the ground or excited state and an inhomogeneous electric field at the nucleus) related to the degree of crystal distortion, thereby magneto-crystalline anisotropy energy (coercivity), and MHF (interaction between the nuclear magnetic dipole moment and a magnetic field) associated with the magnetic moment (saturation magnetization) and inequivalent crystallographic sites, i.e., sublattices.

Mossbauer applications include studying the structure and magnetic properties of nanocrystalline and amorphous materials, core-shell magnetic materials, the interfacial region between ferromagnetic nanocrystallite and amorphous matrix, substituted sites, and magnetic phase transformation. In this paper, we will introduce basic Mossbauer spectroscopy and a detailed interpretation of the Mossbauer spectrum to obtain quantitative magnetic properties.

Abstract ID: 525

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Solar Cells

Keywords: perovskite, perovskite solar cell, high-speed process, solution shearing process, meniscus, perovskite crystallization, crystallization

A study on the meniscus stability of meniscus solution shearing coating for maximizing the crystal size of perovskite at high speed

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Perovskite solar cells are one of the new and renewable energies. Many studies are underway because they have the advantage of being inexpensive in process cost by using inexpensive materials and enabling low-temperature solution processes. To mass-produce large-area perovskite solar cells, a high-speed process must be applied. However, in the case of perovskite materials, when fabricated in a high-speed process, the size of the crystals, which greatly affects the efficiency, tends to decrease, making it difficult to apply mass productio〖n(Roll to Roll process)〗^1.

In this paper, a process study was conducted using the meniscus solution shearing process technology to fabricate a perovskite thin film having a large sized crystal even at high speed. The equipment used is an equipment using a meniscus formed by a capillary phenomenon of a gap between a substrate and a blade, and the stability of the shape of the meniscus is one of the factors that have many influences on the thin film^2. To confirm this, after setting the gap and the blade angle to various values among the process parameters of the equipment, the meniscus shape and the perovskite crystal change accordingly were confirmed. As a result of the experiment, a stable meniscus was confirmed at a blade angle of 3° and a gap of 100㎛, and crystals having a crystal size of 10246.54$\mu m2$ were obtained. However, at a blade angle of 10° and a gap of 500㎛, the meniscus shape became unstable, and it was confirmed that the size of the crystal at this time decreases compared to that of the stable meniscus. Through this study, the optimum process conditions were established to produce a thin film of perovskite with large sized crystals even under a high-speed process of 20 mm/s. Compared with the low speed (~5mm/s) conducted in the previous study, a similar sized crystal was obtained to confirm the possibility of a high-speed process, which has great originality from the previous study

Abstract ID: 526

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Sensors and MEMS: Materials and Devices

Keywords: Metal oxide, Nanowire, Gas sensors, Food quality

Single nanowire chemoresistor as a gas sensor to assess food quality

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The ability to assess the quality of food throughout the production and distribution chain, from producer to consumer, is very important. This allows to reduce food waste, increase the efficiency of the system and avoid problems of food poisoning and consequent health costs. To make this possible you need sensors that are tiny and cheap, but that can assess the quality of food quickly and accurately. Chemoresistive sensors are ideal for this task: they are micron sized, easy and inexpensive to manufacture and read, and are sensitive to a wide range of volatile compounds.

In this specific case, a single tin oxide nanowire was used to evaluate the state of freshness of mackerel fish (Scomber scombrus) over time. The single nanowire sensor measures the concentration of total volatile basic nitrogen (TVB-N), which collects dimethylamine, trimethylamine and ammonia (produced by fish-degrading bacteria). The response of the sensor to the TVB-N was compared with the bacterial population measurements, resulting well correlated with the total vital counts (TVC). The resistive nanosensor therefore proves to be ideal for having a first estimate of the quality of the mackerel (stored at room temperature or in the fridge), which can be obtained non-invasively and in a few seconds

Abstract ID: 527
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Concrete and cementitious composites
Keywords: Concrete, Macrocrack Opening, Gas Permeability

Determination of the Apparent Gas Permeability in a Macrocracked Concrete

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This paper reports on an analysis of an experimental study that aimed to determine the apparent gas permeability in cracked concrete. There is a lack of research on this topic in the international literature, due to the difficulty of performing reliable experimental testing for gas permeability. The principal interest of this work is to present new and reliable experimental results. It also proposes an analysis method for assessing the role of apparent crack opening in the development of apparent crack permeability. The relation between the apparent crack opening and the apparent gas permeability appears relevant in consideration of Poiseuille theory.

Abstract ID: 528

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Electrochemical Supercapacitors

Keywords: Graphene Oxide, Interlayer Interactions; Charge Storage

Effects of Graphene Oxide and Reduced Graphene Oxide Interlayer Interactions on the Charge Storage Mechanism

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Graphene (GP) has been an object of great interest for researchers ever since its isolation from graphite back in 2004. A great many details about the electronic structure and properties of GP has been extensively studied and the knowledge gained has been utilized in fabricating a wide variety of devices. However, to the best of authors knowledge, there has never been a report studying the interlayer interaction (ILI) properties of graphene oxide (GO)/reduced graphene oxide (rGO) composite. Here, we report fabricating GO_GO, GO_rGO, rGO_rGO, and rGO_GO electrodes through screen printing and study their electronic structure and properties through spectroscopic and electroanalytical methods. The electroanalytical techniques used were cyclic voltammetry, Tafel analysis. electrochemical impedance spectroscopy, chronoamperometry, and galvanostatic charging and discharging (GCD). Standard K3[Fe(CN)6] solution of 1 mM concentration was used in investigating the ILI properties. Furthermore, the electrochemical double layer charge storage (EDLC) mechanism for all the systems were investigated through two electrode symmetrical and asymmetrical setups. Though the research is just in its infancy, analysis of the data obtained so far shows the areal capacitance for the symmetric GO_GO, GO_rGO, rGO_rGO, and rGO_GO systems to be 0.74, 3.24, 0.22, and 0.31 mF/cm2, respectively in 1M KCl aqueous solution. For the asymmetrical system the GO_rGO(anode)-GO_GO(cathode) (4.92 mF/cm2) setup showed the highest areal specific capacitance. The operating potential window optimization revealed that GO_rGO and GO_rGO(anode)-GO_GO(cathode) setups could maintain EDLC up to 1V window, while the other setups started showing deviations after 0.7 V window. We intend to thoroughly investigate the ILI process for these four different setups and how they contribute to the EDLC mechanism.

Abstract ID: 529

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanomaterials and Nanotechnology

Keywords: Graphene Oxide, Layer by Layer Assembly, Bisphenol A

Layer by Layer Assembly of Graphene Oxide and Reduced Graphene Oxide for Electrochemical Oxidation of Bisphenol A

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Here, we report fabricating graphene oxide (GO)_GO, GO_reduced graphene oxide (rGO), rGO_rGO, and rGO_GO electrodes through screen printing and study their electronic structure and properties for electrochemical oxidation of bisphenol A (BPA). The electroanalytical techniques used were cyclic voltammetry, Tafel analysis, electrochemical impedance spectroscopy (EIS), and chronoamperometry. The electron transfer mechanism for all the systems were investigated for BPA analyte. Though the research is just in its infancy, analysis of the data obtained so far showed that BPA interacted differently with each of the systems. The BPA oxidation peak current (Ipa) and peak potentials (Epa) for GO_GO, GO_rGO, rGO_rGO, and rGO_GO were determined to be: 1.93 µA @ 0.51 V; 1.47 µA @ 0.5 V; 0.8 µA @ 0.53 V; and 3.6 µA @ 0.5 V; respectively. Tafel slope analysis yielded values of 32.45 mV/dec for GO_GO, 55.4 mV/dec for GO_rGO, 70 mV/dec for rGO_rGO, 90.1 mV/dec for rGO_GO. These different values of Tafel slope indicates that the electron transfer kinetics is different for each of the systems. We intend to thoroughly investigate the interlayer interaction (ILI) process for these four different setups and how they contribute to the electrode/electrolyte interfacial charge transfer process.

Abstract ID: 530

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Metamaterials and Materials for THz, Plasmonics and Polaritons

Keywords: Two-dimensional nano-gratings, surface plasmon resonance, polarization-contrast imaging, azobenzene materials.

Plasmonic imaging using two-dimensional metallic surface relief gratings

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Crossed Surface Relief Gratings (CSRGs) are two-dimensional gratings that result from the sequential exposure of an azobenzene molecular glass thin film to two orthogonal sinusoidal laser interference patterns using a Lloyd mirror interferometer. The resulting large-scale gratings are stable and can be coated with a thin silver layer to permit Surface Plasmon Resonance (SPR). The physical characteristics of the gratings are adjusted during the fabrication process to optimize the excitation of the plasmon at a desired wavelength. In this work, CSRGs are fabricated and used to image and detect localized refractive index variations in inhomogeneous water-based solutions, deposited over them, via polarization-contrast SPR imaging. When a CSRG is placed in between crossed polarizers, incident polychromatic light is transmitted at an intensity level directly and precisely related to the local refractive index of the inhomogeneous solution deposited over the grating. This observation occurs because of the in-plane polarization conversion of the SPR light in between the orthogonal gratings. When viewed with a camera, transmitted SPR light from a monochromatic source enabled the acquisition of polarization-contrast microscopy images of a water and silicon oil mixture placed over the CSRG's surface. Therefore, the intensity of the transmitted monochromatic light across the CSRG, which was placed in-between crossed polarizers, can be directly correlated to the local RI of the solution. This SPR imaging technique will certainly be useful in a variety of medical applications because all the background light is cancelled due to the crossed polarizers and only SPR light is transmitted and recorded.

Abstract ID: 531
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Design and application of composite structures
Keywords: Cucurbituril, coumarin, piperazine, benzimidazole, photoinduced electron transfer, indicator displacement assay, pKa shifts

Coumarin/CB7 Supramolecular PET Fluorochrome for Detection of Carnosol by Stimuli-Responsive Dye Displacement and pKa Tuning

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In recent years, the number of indicator displacement assays (IDAs)[1] has increased as an eminent strategy for changing a synthetic receptor (host) into an optical sensor. In a conventional IDA, an indicator (dye) is first permitted to reversibly bind a host, before being dislodged from the host by a competitive analyte (drug) and thusly the strategy regulates an optical signal despite the analyte and the host are both spectroscopically inactive. It is quite crucial that the indicator and analyte have similar affinity for the receptor.[2–6]

A new fluorescent dye (4PBZC) comprises of coumarin, piperazine and benzimidazole (BZ) was designed, prepared and complexed to cucurbit[7]uril (CB7) to detect carnosol (CAR) anticancer drug in sub-nanomolar concentrations utilizing the supramolecular indicator displacement assay (IDA) strategy, the CB7-assisted pKa shift and the CB7-retarded photoinduced electron transfer (PET) process. The 2:1 host−guest complexation was confirmed by UV−visible absorption, fluorescence and proton NMR spectroscopy, which confirm binding to 4PBZC via the BZ and coumarin moieties. Also, CB7 preferentially binds the indicator dye via the protonated BZ group compared to the neutral BZ group, demonstrated by a high 2:1 binding constant (e.g., K = 5.5 × 106 M−1) of the complex in its protonated form, which led to an increase in the pKa of the BZ moiety by ca. 3.0 units after the addition of CB7. In the aqueous solution under pH of 6, switching the emission signals between 4PBZH+C/CB7 (ON state) and CAR/CB7NPs (OFF state) was achieved by displacement of the protonated dye from the cavity of CB7 by the CAR analyte. An efficient sensor was fabricated for the highly sensitive detection of CAR in aqueous solution at pH 6 with a low-detection limit (LOD) of 0.06 ng/mL (0.2 nM).

Abstract ID: 532

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: Piezoelectric Energy Harvesting, Smart Materials, Energy Conversion, FE Simulation, Coupled Problem

Nonlinear Finite Element System Simulation of Piezoelectric Energy Converters

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A piezoelectric vibration-based energy harvester (PVEH) is composed of an electromechanical structure along with an energy extraction circuit. The objective of such a device is converting otherwise unused mechanical energy to electrical energy to power e.g. wireless sensors. The piezoelectric effect, used as the energy conversion principle, describes the appearance of electrical voltage when the piezoelectric material is mechanically deformed and vice versa. In an energy harvesting application the electromechanical structure and the electrical circuit have an influence on each other. This necessitates the accurate modeling of both parts and their interactions[1]. However, until now all finite element (FE) based methods reported in literature, which are not coupled to a circuit simulation software, are limited to linear circuit elements and passive electrical interfaces. The FE based methods, which are combined with an external circuit simulation tool, consider only linear electromechanical structures or the coupling between the electromechanical structure simulation and the electric circuit simulation is not very efficient. To overcome the mentioned drawbacks of existing FE methods for PVEH we developed a FE based approach, which can simulate nonlinear behavior of electromechanical structures as well as nonlinear and active electric circuits [2]. The influence of the circuit on the electromechanical structure is considered via the vector of external forces and an implicit time integration scheme is applied. The proposed method allows for consistent and efficient simulations of the complete possibly nonlinear PVEH using only one software tool.

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Abstract ID: 533

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Solar Cells

Keywords: Nano composite; Polyaniline; dc conductivity; adsorption; Solar

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Researchers have used conducting polymer polyaniline, Polypyrrole for energy and environment applications. Here nanocomposite material was developed with nano SnO2, TiO2 and polyaniline by in-situ polymerization techniques. This material was characterized by Scanning Electron Microscopy (SEM) and dc conductivity, Keithley equipment. The material was also utilized for the adsorption purpose for chromium from Potassium dichromate (K2Cr2O7) solution and characterized with UV absorption coefficients.

Key words: Nano composite; Polyaniline; dc conductivity; adsorption

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Abstract ID: 534

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Thin Films and Nanomagnets

Keywords: RF and DC sputtering, Titanium nitride, TiN-Si3N4 nanocomposite, Stoichiometry-dependent properties

Titanium nitride-based multi-functional thin films

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The most important applications of Titanium Nitride (TiN) based thin films are in the production of load-bearing components and the semiconductor industry as diffusion barriers for metals. In this paper, it is shown that TiN thin films display several more functionalities in addition to attractive mechanical and electrical properties. TiN thin films are grown by RF and DC magnetron sputter deposition from a Ti target in Ar+N2 or pure N2 atmosphere. By controlling the process, amorphous, nanocrystalline or crystalline TiNx (x<1) films are obtained. One of the most important contributions of our group was the development of a patented process to stabilize single phase Ti2N thin films [1]. The properties of these thin films include a large band gap and medium hardness. The evolution and stability of this phase is critically dependent on process parameters and film thickness. It is also established that TiN exhibits a nitrogen-stoichiometry-dependent reflectivity minimum centred around 530 nm. Calculations of optical constants indicate that this feature corresponds to a surface plasmon resonance (SPR) and is observed in both undoped and Nb-doped TiN thin films [2, 3]. TiN thin films are, thus, a cost-effective alternative to gold thin films that are normally used in SPR-based sensing applications. This study was extended to investigate the electrical, mechanical and optical behaviour of TiN-Si3N4 nanocomposite thin films. Uniquely, these films are grown on Phynox (Co-Cr-Ni) alloy and IN718 substrates and display excellent conductivity, hardness and high optical reflectivity [4]. Thus, this work expands the range of applications of TiN thin films into the electrical, optical, opto-electronic and sensing domains by controlling non-stoichiometry and doping.

Abstract ID: 535

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Photonic devices and applications

Keywords: radiative cooling, wearable devices, thermal management, oximeter

Passive radiative cooling structures for applications in outdoor-useable, patch-type wearable devices

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For wearable devices, thermal management should be provided for accurate signal acquisition as well as thermal comfort. However, outdoor solar energy gain has restricted the efficiency of some wearable devices, resulting in inaccurate data acquisition and skin burn effect [1]. Meanwhile, recently reported passive radiative coolers has been considered as a candidate for an effective cooler with no electricity in many outdoor applications [2-5]. Herein, we present wireless/battery-free and thermally regulated patch-type tissue oximeter (PTO) with radiative cooling structures, which can measure tissue oxygenation under sunlight in reliable manner and will benefit athlete training. To maximize the radiative cooling performance, we introduce a nano-/micro-voids polymer (NMVP) by combining two perforated polymers to both reduce sunlight absorption and maximize thermal radiation. The optimized NMVP exhibits sub-ambient cooling of 6 °C in daytime under various conditions such as scattered/overcast clouds, high humidity, and clear weather. The NMVP-integrated PTO enables maintaining temperature within ~ 1 °C on the skin under sunlight relative to indoor measurement, whereas the normally used, black encapsulated PTO shows over 40 °C owing to solar absorption. The heated PTO exhibits an inaccurate tissue oxygen saturation (StO2) value of ~ 60 % compared with StO2 in a normal state (i.e., ~ 80 %). However, our thermally protected PTO presents reliable StO2 of ~ 80%. This successful demonstration provides a feasible strategy of thermal management in wearable devices for outdoor applications.

Abstract ID: 536

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Computational modeling and simulation for energy storage and conversion devices
Keywords: Cattaneo-Christov heat and mass flux theory; Optimal convergence control parameter; Auxiliary function; Homotopy; New technique.

New Technique for the dynamic analysis and numerical simulation of Cattaneo-Christov heat and mass flux model

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Cattaneo-Christov heat and mass flux theory is documented to remove the restriction implemented by Fourier law on energy and concentration equations to parabolic type equations. Steady two-dimensional hydromagnetic mixed convection flow of Maxwell nanofluid suspended with nanoparticles controlled through stretching sheet is scrutinized. CC-model is followed for heat transfer carrying the Brownian motion, thermophoresis, and viscous dissipation. Double stratification is observed.

Gyrotactic microorganisms are distributed for which water is taken as base fluid. Darcy Forchheimer's law is incorporated for porous medium. The self-similarity variables have been applied to convert the modeled equations into a set of non-linear coupled differential equations. These non-linear differential equations have been treated through a new analytical technique. The new technique consists of Homotopy, optimal convergence control parameters, auxiliary functions. The solution of the coupled

problem through this new method and its fast convergence is mainly focused on this work. The effect of physical parameters that appears in the problem is shown graphically and discussed. Finally, the obtained results are compared with a numerical (ND-Solve) method to authenticate the code of the applied technique. The physical and numerical agreement of these two methods has been shown.

Keywords: Cattaneo-Christov heat and mass flux theory; Optimal convergence control parameter; Auxiliary function; Homotopy; New technique.

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Abstract ID: 537

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Optical properties of metals and non-metals

Keywords: Fluorescence, Phosphorescence, Molecular Conformation

Achieving Conformational Control in RTP and TADF Emitters by Functionalization of the Central Core

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Nowadays, a manifold of fluorescent emitters has been developed for optoelectronic applications including organic light emitting diodes,1 sensing,2 probes for fluorescent imaging3 and optical thermometry.4 However, most of the emitters follow the singlet decay channel only, thus limiting the efficiency. Therefore, there is a need for alternative ways to harvest both singlet and triplet excited states. Thermally activated delayed fluorescence (TADF) is currently the leading strategy offering internal quantum efficiency (IQE) of 100% using purely organic emitters.5 In turn, efficient room temperature phosphorescence (RTP) can be realized when the molecular vibrations causing non-radiative T1→S0 relaxations are suppressed and efficient intersystem crossing (ISC) from S1 to T1 is promoted.6

The current work presents a new molecular design approach aimed at preventing the formation of multiple axial and equatorial conformers while employing the phenothiazine donor in a D-A-D system with the 9,9-dimethyl-thioxanthene acceptor unit. By introducing pertinent substituents onto the acceptor and altering the linking position of the donor moiety efficient RTP emitters with solely equatorial conformation were obtained. Moreover, functionalization of the thioxanthene with electron deficient groups resulted in a negligible ΔEST, enhanced reverse ISC (RISC) rate and efficient yellow TADF. A thorough photophysical investigation is provided. Theoretical calculations assist the understanding of the observed results.

Key Words: Fluorescence, Phosphorescence, Molecular Conformation

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Abstract ID: 538

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Solar Cells

Keywords: Solar Cells, Organic Light Emitting Diodes, Platinum(II), Copper(I), Lanthanide(III)

Poly-ynes, Poly(metalla-ynes), Coordination Complexes and Polymers for Opto-Electronic (O-E) Applications

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The quest for high performance opto-electronic (O-E) devices for sustainable energy have led to the development of new generation efficient, cost-effective, and lightweight solar cells (SCs) and organic light emitting devices (OLEDs) based on conjugated organics, organometallics, coordination complexes and polymers.1 This has been possible largely due to the diverse modern synthetic protocols generating new functional materials with easily tunable properties such as extended π-conjugation, good absorption profile, photoluminescence (PL) etc. A wide range of conjugated organic, organometallic and coordination polymers as well as their model compounds are extensively investigated in our laboratory (Chart 1). The first series consists of Pt(II) poly-ynes incorporating a wide variety of conjugated carbocyclic, hetero-cyclic and mixed hetero-cyclic spacers. Pt(II) poly-ynes are excellent phosphorescent materials with long-lived triplets promoting charge generation and enhancing efficiency of the O-E devices. The second series is comprised of organic co-polyynes using phenothiazine (PTZ) as a common motif. The materials have shown promise for application in bulk hetero-junction (BHJ) SCs and polymer LEDs. The third series is comprised of metal organic framework (MOF) materials, self-assembled from ferrocenyl ethynylpyridine and Cu(I) halides. A range of dinulear arylethynylpyridinyl Cu(I) halide phosphine complexes (aryl = carbocyclic and heterocyclic spacers) bearing anchoring carboxyl acid groups have been assessed as dyes in DSSCs. The fourth series consists of luminescent coordination complexes of trivalent lanthanide ions. The complexes have been utilized as emitting layer in the OLEDs to fabricate red, green and even white OLEDs. The design, synthesis, chemistry and photophysics of these materials will be reviewed with structural analysis of their model compounds. Fabrication of SCs and OLEDs incorporating these novel materials and evaluation of their device performance will be presented.

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Members of the Materials Research Group

Prof. Paul R. Raithby, Dr. Nawal Al-Rasbi, Dr. Mohamed Al-Suti, Dr. Rashid Ilmi, Dr. Ashanul Haque.

Abstract ID: 539
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Polymeric composites
Keywords: Shape Memory Polymer, Epoxy Polymer, Nano Carbon Material, Composites

Curing Behavior Analysis and Performance evaluation of Epoxy based Shape Memory Polymer Composites

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Shape Memory Polymers (SMPs) is a polymer compound with property of remembering the original form and returning to the original form by specific external stimulations such as heat, light, current, and magnetic field. SMPs has a smaller density than shape memory alloys, so it is easy to realize light weight characteristics, and has relatively excellent shape memory characteristics. in addition, it can be applied in various fields due to its low price and good formability. However, the domestic research on the shape memory materials is mainly carried out on the academic scale, mainly on metal-based alloys, and it is in the early stage. In this study, we tried to find optimized shape memory polymer composites and shape memory performance by serval fillers, hardeners, and curing conditions. In addition, by adding nano-carbon materials such as graphene, CNT and etc., the mechanical properties data of the composites with improved shape memory performance were secured.

Abstract ID: 540

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanomaterials and Nanotechnology

Keywords: Ionic Liquids, Colloidal Systems, Nanoreactors, Advanced Materials

Ionic Liquids Based Colloidal Solutions as Nanoreactors for Advanced Materials

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Room temperature ionic liquids (RTILs) are the organic analogues of inorganic molten salts with melting temperature <100oC [1]. Being ionic in nature, these compounds are versatile in terms of solvent properties such as low volatility, high thermal stability, wide liquid range and good solvating ability. In view of flexibility of choice of cations or anions, RTILs can designed as low viscosity media suitable for self-assembling of amphiphile molecules or also can also be designed as surfactants by incorporating amphiphilic character in either cation or anion or in both the constituents. Therefore, with extraordinary properties it has been possible to include RTILs as media or as surfactant or both for preparation of colloidal formulations/self-assembled structures [2]. Such structures are highly thermally stable and can be used as recyclable templates for preparation of shape/size controlled nanomaterials/quantum dots/metal organic frame works (MOFs), carbon dots (CDs) and hybrid materials [3,4]. We have constructed a stable ionic liquid colloidal system, where low viscosity ethyl ammonium formate IL is used as medium, R (+) limonene as non-polar medium, and bio-based surface active Choline[AOT] as an amphiphile. Self-assembled structures, thus constructed, have been utilized as recyclable nanoreactors for synthesis of a variety of shape and size controlled MOFs viz. HKUST-1, Uio-66-NH2, ZIF-8, and MIL-53(Al)-NH2 at room temperature in a generalized approach. The synthesized MOFs have been studied for gas adsorption and preparation of composite membranes for mixed salt separation applications.

Key Words: Ionic Liquids, Colloidal Systems, Nanoreactors, Advanced Materials

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Abstract ID: 541

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: All solid-state batteries
Keywords: lithium dendrites, short circuit, residual compressive stress, stress corrosion cracking

A New General Paradigm for Understanding and Preventing Li Metal Penetration through Solid Electrolytes

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The use of lithium (Li) or sodium (Na) metal anodes together with highly ion-conductive solid electrolytes (SEs) could provide batteries with a step improvement in volumetric and gravimetric energy densities. Unfortunately, these SEs face significant technical challenges, in large part because Li and Na dendrites can penetrate through SEs, leading to short circuits. The ability of such a soft material (Li or Na metal) to penetrate through ceramic is surprising

from the point of view of models widely used in the Li-battery field. We introduce a concept, new to the battery field, for preventing penetration of lithium dendrites through SEs by putting the SE surfaces into a state of residual compressive stress. For a sufficiently high compressive stress, cracks have difficulty forming, and cracks that do form are forced to close, inhibiting dendrite penetration. This approach is widely used to solve commercially important stress corrosion cracking problems in metals and static fatigue problems in ceramics and glasses (e.g., Gorilla Glass). However, the technique will not be useful for SEs if the Li-ion transport rate through a SE is substantially reduced when the SE is under compression. Our molecular dynamics calculations for Li-ion transport through a common SE demonstrate that the introduction of even very high residual compressive stresses (10 GPa) has only a modest effect on Li-ion transport kinetics, suggesting that this approach is viable and capable of providing a new paradigm for developing high-performance and mechanically stable SEs.

Abstract ID: 543

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nano-Magnetic, Magnetic Memory and Spintronic Materials

Keywords: Metal-insulator nanocomposites, Extra ordinary Hall effect, Tunneling magneto resistance, Field emission, Exchange bias, Density functional theory

Embedded metal nanoparticles: shape engineering, electronic and magnetic properties, an experimental and theoretical investigation

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Metal nanoparticles (NPs) embedded in a thin dielectric medium is a class of materials those have shown promising applications in various scientific and technological fields. Ferromagnetic metal-insulator (FM-I) granular films have attracted a considerable attention because they exhibit a wide variety of interesting properties in magnetism and magneto-transport, which suggest their attractive applications like information storage, shielding and bit writing at high frequencies, MR sensors and read heads, high sensitivity Hall sensors, field emission and solar energy applications.

In the present work, Ni: SiO2 (Ni nanoparticles embedded in SiO2 matrix) and FeCo: SiO2 (FeCo nanoparticles embedded in SiO2 matrix) granular films of various metal atomic fraction (x) have been prepared by Fast atom beam (FAB) sputtering technique and their structural, electrical, magnetic, magneto transport and field emission properties have been studied.

The following results have been highlighted in the talk: (i) Enhanced extra ordinary Hall effect (EHE) in Ni-SiO2 films, (ii) Tunneling magnetoresistance in FeCo-SiO2 films, (iii) exchange bias effect in FeCo-SiO2 films and (iv) enhanced field emission current density from shape engineered FeCo NPs embedded in SiO2 matrix. An in-depth analysis of the results have been carried out using state of the art experimental techniques and density functional theory (DFT) based calculation. Finally, prototypes developed using these materials will be shown.

Keywords: Metal-insulator nanocomposites, Extra ordinary Hall effect, Tunneling magneto resistance, Field emission, Exchange bias, Density functional theory

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Abstract ID: 544
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Multifunctional composites
Keywords: Magnetoelectric Effect, Magnetoelectric Composite, Built-in Deformation

Direct magnetoelectric effect in Two-layer ceramic composites based on Ferrimagnet Mn0.4Zn0.6Fe2O4 and Ferroelectric PbZr0.53Ti0.47O3

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Under different experimental conditions, the direct magnetoelectric (ME) effect was studied in two-layer composites prepared both by joint sintering of layers of powders of ferrimagnet Mn0.4Zn0.6Fe2O4 (MZF) and ferroelectric PbZr0.53Ti0.47O3 (PZT) and by gluing layers pre-sintered from powder materials of MZF and PZT. The purpose of such studies was to determine which of the factors, the mutual doping of the phases [1], that took place during the high-temperature sintering of layers of MZF and PZT powders, or the adhesive joint, less weakens the ME effect in the composites.

Abstract ID: 545

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Theoretical and Computational Magnetism

Keywords: Magnetocaloric effect, elastic properties, rare-earth transition metal compounds.

Elastic, Magnetothermal and Magnetocaloric Effect of YFe3 and HoFe3 Compounds

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We report on the temperature and field-dependence of the magnetothermal properties and magnetocaloric effect in YFe3 and HoFe3 compounds. The mean-field theory and the ab initio calculation, using the Density Functional Theory (DFT) as implemented in the Wien2k code, were used. The calculations of the magnetization, magnetic heat capacity, magnetic entropy and the isothermal change in entropy ΔSm were performed using the two-sublattice model of the mean-field theory. For calculating the lattice, electronic specific heat and the corresponding entropies, and subsequently the adiabatic change in temperature ΔTad, we performed the ab initio calculation to determine the Debye temperature ΘD and the density-of-states at Ef. The bulk and shear moduli of YFe3 are in the 95-236 GPa range, the average speed of sound is ≈ 4167 m/s, and the Debye temperature is ≈ 500 K. The trapezoidal method was used to calculate ΔSm, in fields up to 60 kOe, and at temperatures up to and beyond the Curie temperature for both compounds. The maximum values, in a 60 kOe, of ΔSm for YFe3 and HoFe3 are about 1.3 and 0.25 J/mol. K respectively. The temperature and field dependences of the magnetothermal properties and of ΔSm and ΔTad show that the ferro/ferrimagnetic to paramagnetic phase transition, in these two compounds, is a second-order-phase-transition (SOPT). The Arrott plots and the universal curve were calculated to provide further checking the type of magnetic phase transition involved in these compounds.

Abstract ID: 546

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Functionally graded composite materials and structures

Keywords: Buckling, Combined loads, Cutouts, First ply failure, Load interaction curves, Postbuckling

Buckling and Postbuckling responses of composite plates under combined in-plane loads

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The buckling and postbuckling responses of functionally graded hybrid composite plates subjected to combined in-plane uniaxial compression and in-plane shear loads are investigated numerically. The finite element analysis-based software ABAQUS has been used for the numerical study. Eigen buckling analysis and Tsai-Hill failure criterions are used to determine critical buckling and first ply failure loads, respectively. Functionally graded composite plates with and without cutouts are considered for the study. Five different shapes and three different sizes of cutouts at the center of the plate have been taken to examine the response under the combined in-plane loads. Effect of (0/90)4s, (+45/-45)4s, and (+45/-45/0/90)2s fiber stacking sequences are also examined and load interaction diagrams are presented for combined in-plane uni-axial compression and in-plane positive and negative shear loads. It is concluded that the diamond-shaped cutout of small size among the cutouts performs better in terms of buckling and first ply failure loads of the plates under compressive loads combined with negative in-plane shear load. The (+45/-45)4s stacking sequence has the highest buckling and failure loads in comparison to other layup sequences.

Abstract ID: 547

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Spintronic Effects and Devices

Keywords: antiferromagnets, spintronics, Cr2O3

Nanomagnetism and spintronics of Cr2O3 thin-film magnetoelectric antiferromagnets

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Thin film magnetoelectric antiferromagnets (AF) is a viable material science platform for prospective high speed and energy efficient spintronic devices for memory and logic applications. To explore their application potential, it is necessary to understand modifications of the magnetic properties of AF thin films with respect to their bulk counterparts. Here, we will discuss spintronics, magnetometry and microscopy of bulk α-Cr2O3 single crystals [1] and relate them to the properties of α-Cr2O3 thin films [2-5]. In transport experiments, we access the magnetic state of the Cr2O3 relying on the spin Hall physics in a Pt thin film brought in proximity to the insulating antiferromagnet [2-4]. The analysis of the transport data is backed up by the real space imaging of AF domain patterns using NV microscopy [1,5]. Considering grainy morphology of thin films, we address questions regarding the change of the intergranular exchange [5], criticality behavior and switching of the order parameter [2] and physics of the readout signal in α-Cr2O3 interfaced with Pt [3]. In particular, the possibility to read-out the antiferromagnetic order parameter all-electrically enables a new recording concept of antiferromagnetic magnetoelectric random access memory (AF-MERAM) [3]. Furthermore, relying on the elasticity of antiferromagnetic domain walls in Cr2O3 single crystals and exploring their efficient pinning at lithographically defined mesa structures, the concept of domain wall based antiferromagnetic memory was put forth [1].

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Abstract ID: 548

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Design and application of composite structures

Keywords: Copper/Carbon Nanotube Composites, Electric Conductors, Lightweight

Developing Lightweight Homogeneously Mixed Heat- and Current-stable Cu/Carbon Nanotube Composite Electric Conductors

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We present our progress with developing homogeneously mixed copper-carbon nanotube composites (Cu/CNT) lighter than copper with rivalling electrical conductivities as well as heat and current-stabilities. Such materials are expected to function as more durable lightweight copper-alternatives in aircraft/automobile electrical wirings for improved weight-reduction and fuel-efficiencies as well as in micro-interconnects for smaller more powerful electronics [1]. To demonstrate macro and microscale applicability, we fabricated Cu/CNT with excellent performances in a variety of structures including cm-scale wires and microscale via-like structures by Cu-electrodeposition of CNT templates [2-6]. Irrespective of structure, our composites show densities <5.2 g/cm^3 and are at least 2/3rd as light as copper. Such low densities could be achieved by tuning composite fabrication to incorporate high nanotube vol% (>40%) with homogeneous CNT-Cu mixing. Room temperature electrical conductivities of our lightweight Cu/CNT are ~ 1-4 × 10^5 S/cm competitive to that of pure copper (5.9 × 10^5 S/cm). The temperature stable conductivity of our composites is reflected by temperature coefficients of resistivity (TCR) as low as 10% that of copper. In terms of current stability, our Cu/CNT's current carrying capacities (CCC) surpass that of copper. Our composites also show better thermal expansion stability with coefficients of thermal expansion (CTE) ~ 4-7 ppm/K, closer to Si-CTE (~3 ppm/K) than Cu-CTE (~17 ppm/K). Besides demonstrating Cu/CNT's promise as a Cu-substitute, we will discuss the various factors (Cu and nanotube spatial distribution, nanotube attributes, metal/nanotube interface, etc.) that affect composite properties to provide pointers for Cu/CNT performance tailoring.

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Abstract ID: 550

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Multiscale Modeling in Mechanics and Composite Materials

Keywords: Composite Materials, Multiscale Modelling, Deformability, Modulus of Elasticity, Layer Model

Layer models in predicting of Composites' deformability

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Regulation and prediction of composites deformability is the important problem in providing calculated limits of structures deformations under mechanical and thermomechanical load.

Composite structure topology is discrete. But topological solution in modelling of structure deformability can include variations of elements' discreteness and infinity. Due to the structure's topological transformation by the method of flat cross-section projection the composites elements in perpendicular to load direction were represented as infinite (graphical abstract). Thus, the composite deformability layer model efficiency was supposed. Infinite elements in layer model of discrete composite structure are intermittent layers of aggregate and matrix. Aggregate is discrete element topologically represented in model as infinite in cross-load direction. The matrix layers depending on composite type can be the binder and contact to aggregate inter-transition zone (ITZ) (Type L-I), the binder only (Type L-II), the ITZ only (Type L-III).

Developing a calculation model of the composites' deformative properties, the dependence of the elastic modulus on the layer model with the number of layers i=n, the elastic modulus of the layer E_i and the relative thickness of the layer δ_i was proposed.

All layer model variations were researched with taking into account the type of composite structure. Analyze included heavy concrete as a type L-I, lightweight concrete as a type L-II, glassed polymer as a type L-III. Efficiency of all layer model variations were proved. It made possible to calculate elasticity modulus of cement and polymer composites depending on materials' contents in mix composition.

The layer modelling is worked out in development of entropy-topological conception of composite structure forming and analysis. The conception is aimed on definition of stress and temperature relations with composite deformability depending on mass and energy entropy. This is represented as a function of topology that includes in massive of points and coordinates massive of masses and inner chemical, physic-chemical or heat energy.

Abstract ID: 551

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Photocatalytic and electrochemical water splitting
Keywords: Photothermal catalysis, Hydrogen, Nanomaterials, Titanium Suboxide, Sonohydrothermal

Engineering of low-cost and environmentally benign catalysts for thermal-assisted photocatalytic hydrogen production

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Conversion of solar energy into hydrogen via photocatalytic splitting of water is an alternative sustainable process of paramount interest for clean energy storage. In this view, preparation of stable and nontoxic catalysts from non-precious elements showinghigh photocatalytic activity under solar light irradiation is of great importance. Herein, we provide new insights into the design of Ti@TiO2 core-shell photocatalyst with advanced photothermal activity in the process of hydrogen production from aqueous solutions of glycerol. Ti@TiO2 nanoparticles have been obtained by sonohydrothermal (SHT) treatment of titanium metal nanoparticles in pure water. SHT process based on simultaneous hydrothermal and ultrasonic treatment has been proven to be effective for the synthesis of nanocrystalline materials with advanced properties.1,2 In general, acoustic cavitation in hydrothermal solutions accelerates the crystallization and improves the catalytic performance of nanocrystalline metal oxides. In this study, we found that variation of SHT temperature allows controlling nanocrystalline TiO2 anatase shell on Ti0 surface. At 100<T<150°C formation of TiO2 nanoparticles occurs mostly by crystallization of Ti(IV) amorphous species and oxidation of titanium suboxide Ti3O presented at the surface of Ti0 nanoparticles. At T>150°C, TiO2 is also formed by oxidation of Ti0 with overheated water. Kinetic study highlights the importance of TiO2 nanocrystalline shell for H2 generation. Electrochemical impedance spectroscopy points out more efficient electron transfer for Ti@TiO2 nanoparticles in correlation with photocatalytic data. The activation energy (Ea=32±2 kJ·mol-1) assumes that photothermal effect arises from the diffusion of glycerol oxidation intermediates or from water dynamics at the surface of catalyst. Interesting that under the heating photocatalytic H2 emission is observed even in pure water in the presence of Ti@TiO2 nanoparticles.

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Abstract ID: 552

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Functionally graded composite materials and structures

Keywords: Keywords: Functionally Graded Composite, Reciprocating wear, High temperature, Coefficient of friction

High Temperature Linear Reciprocating Wear Behavior of Al-Mg2Si in-situ Functionally Graded Composites

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Higher fuel economy and reduction in emissions demands design improvements in contemporary automotive engine components which need to satisfy two essential tribological property requirements- a good wear resistance and low coefficient of friction. The commonly employed Al alloys like A356 and A319 do not satisfy these tribological property requirements. In emerging functionally graded (FG) composite materials, graded microstructure and compositions are possible to be developed. The large volume percentage of hard reinforcing phases segregated in the surface layer result in excellent wear properties and at the same time gradual depleting of reinforcing phase away from the surface leads to betterment in ductility and toughness. Functionally graded aluminum based Mg2Si reinforced composites is a prospective material for different advanced applications. Graded Al-Mg2Si composite could be fabricated by in-situ reaction between Mg and Si in molten Al-Si-Mg alloy by centrifugal casting technique. Mg2Si particles are segregated at the inner surface of tubular casting due to lower density compared to that of molten aluminum [1]. The reinforcing phase Mg2Si has a high hardness, light in density, high melting temperature, low coefficient of thermal expansion and a moderately high elastic modulus. The automotive engine components like cylinder liners are subjected to a scuffing type of wear by the continuous movement of piston against it at a considerably elevated temperature of around 1500C to 2000C. Hence, high temperature linear reciprocating wear characteristics are important for successful employment of this FG composite. However, to the authors' knowledge no published information is reported yet on the high temperature reciprocating wear characteristics of hypoeutectic Al-Mg2Si graded composites with percentage variation in Mg and its interrelation with microstructural features. The high temperature reciprocating wear characteristics have been evaluated in the present study for the inner surface of some T6 treated A356-Mg2Si functionally graded composites with change in %Mg (2.5, 5, 7.5 and 10 wt%). The wear loss continuously decreases as %Mg is increased from 2.5% to 7.5% and rises little bit with 10%Mg. The FG composite with 7.5%Mg shows the best combination of wear characteristics and coefficient of friction.

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Abstract ID: 553

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Spintronic Effects and Devices

Keywords: ultrasound injection, yttrium iron garnet, neutron scattering

Neutron scattering on yttrium iron garnet under ultrasound injection

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In yttrium iron garnet YIG [1], the spin current has been observed as a spin Seebeck effect under a temperature gradient [2] and ultrasound injection [3,4]. The neutron scattering on a YIG single crystal under ultrasound injection has been performed by using DNA (BL02) with high energy resolution, to study the spin pumping effects on magnetic Bragg peak and magnon. At room temperature, a magnetic Bragg peak at (220) was only slightly enhanced by the ultrasound injection, whereas the effect was significantly increased at low temperatures. The peak width in energy was also increased depending on the applied voltage at the LiNbO3 transducer. In YIG, so far, an anisotropic magnetic capacitance effect is observed at low temperatures [5]. In this project, we accidentally discovered that the Zeeman energy gap diminished significantly at low temperatures only under a magnetic field along the [111] axis in the same temperature range [6,7]. Our recent result on Er3Fe5O12 will also be presented. This anomaly was confirmed by specific heat and magnetization. The spin-lattice coupling will be discussed as to their possible origins of the anomalies. This work has been performed at DNA(BL02) of J-PARC MLF under the proposals 2017L0301, 2014B0157, 2015I0002, and 2016A0318.

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Abstract ID: 554
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Nanocomposites
Keywords: Quantum Dots, Nano, Liquid Crystals

Electric conductivity of CdSeZnS quantum dots dispersed in liquid crystals.

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Liquid crystals (LC) are continuous, organized and flexible structures that can host a large variety of particles. The smallest particles known so far, nanoparticles, are quite interesting for many applications so a deep understanding is needed to use them efficiently.

Unlike isotropic dispersions, liquid crystals allow us to obtain a reproductible structures that can be controlled by a external fields and provide valuable information about the electric or magnetic properties of inserted nanoparticles. A key point in this process is to identify and describe the interaction forces between the surface of the particle and the surrounding molecules. So far, we developed theoretical models and experimental studies [1], [2] for the electric response (i. e. Freedericksz transition) and dynamic behavior (relaxation times) of liquid crystal composite with quantum dots. This research helped us to understand the electric conduction process in liquid crystal cells with small amount of CdSe/ZnS quantum dots. By adjusting the quantum dots concentration, temperature and applied voltage and after comparing the results with theoretical

expectation, we obtained the electric parameters of quantum dots but also provided a procedure that can be used for other similar mixtures and particles. The may help the development of high performance electro-optic devices and improve the impact of technologies in research, industry and everyday life.

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Abstract ID: 555

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Graphene, Mxenes and other two-dimensional materials for biomedical and healthcare applications

Keywords: magnetic nanoparticles, drug targeting, magnetic field gradient

Surface functionalization of magnetic nanoparticles for magnetically driven passage through eye tissues for magnetic drug targeting

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If a pharmaceutical agent has to be applied into a patient's eye, for example because of a disease of the retina, a drug administration by an intravitreal injection directly into the vitreous body is a common and very effective strategy. This injection causes severe risks and discomfort for the patient, so that an alternative strategy to target the drug would be very beneficial. Therefore, we are evaluating the possibility of magnetic drug targeting into the eye by using magnetic nanoparticles (MNP) to which the drugs can be linked.

Magnetic nanoparticles with an optimized multicore structure were selected for this application by evaluating the stability against agglomeration of MNP with different functional coatings (e.g. different dextranes, starch, citric acid, PEG) in water for injections, physiological sodium chloride solution, and biological media like artificial tears fluid. From these investigations, starch turned out as the most promising coating material because of its stability in saline fluids due to its steric stabilization mechanism.

To evaluate the passage of MNP through the sclera and cornea of domestic pig (sus scrofa domesticus) eye tissues, a 3D printed setup consisting of two chambers (reservoir and target chamber) separated by the eye tissue, was developed. With a permanent magnet array, emulating the 20 T/m field gradient of a superconducting targeting setup promising for such targeting as found in simulations, experiments aiming on a magnetically driven transport of the MNP from the reservoir chamber into the target chamber via the tissue were performed. The resulting MNP concentration in the target chamber was determined by means of quantitative magnetic particle spectroscopy (MPS). It was found that, none of the tested particles passed the cornea, but starch coated particles can pass the sclera with a rate of about 5 ng/mm2 within 24 hours. These results open the door for a future magnetic drug targeting to the eye.

Abstract ID: 556

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Dielectric materials

Keywords: Novel Electrical Insulation, Multilayer, High Voltage, Multifunctionality, Lightweight

Progresses in Developing Micro-Multilayer Multifunctional Electrical Insulation (MMEI) System for High Voltage Applications

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Development of the novel patented high voltage insulation system, namely micro-multilayer multifunctional electrical insulation (MMEI) was continued particularly for the future hybrid or all electric aircraft applications. Initially, the concept and feasibility of the MMEI system was successfully demonstrated with its exceptionally high dielectric breakdown voltage, reaching 91% highest increase over the Kapton® PI film alone at the same overall thickness when the multilayer structure of the Kapton® PI films and binder layers such as PFA was optimized in terms of individual film thickness and layer configuration, Figure 1. Overall, MMEI structures outperformed any other SOA polymer insulation materials or commercial system such as Teflon-Kapton-Teflon (TKT). Since then, further optimizations and improvement of the system were pursued with specific emphasis on multifunctionalities such as moisture blocking, partial discharge (PD) resistance, durability, etc. Efforts have been also continued to identify the controlling mechanisms for the major improvement in dielectric strength of the MMEI structures via 3-dimensional dielectric failure mode analysis, Figure 2. At the same time, significant progresses have been made in scaling up the MMEI structures and assessing their commercial applicability and manufacturability in full-scale 3-dimensional prototypes of electrical components, such as power cables and bus bars. Overall progresses on the MMEI development to date will be presented in this paper.

Abstract ID: 557

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanoparticles, Nanowires, and 3D Structures

Keywords: Silicon, Nanowires, Thermoelectricity, Heat harvesting

Silicon Nanopillars by Metal-Assisted Chemical Etching: From Active Thermoelectric Components to Nanoresonators

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Single-crystalline silicon is well known to be a poor thermoelectric material because of its large thermal conductivity k (ca. 150 W/mK at 300 K). This notwithstanding, making silicon an effective thermoelectric material would deeply impact thermoelectric technology due to its large geo-availability, low cost and compatibility with electronics. This has motivated a large effort to reduce single-crystalline Si k, making extensive use of the nanotechnology toolbox.

Single-crystalline Si nanowires (NWs) are well known to display k values down to 5 W/mK because of the inelastic scattering of phonons at wire walls. Since electron scattering is instead coherent, thermoelectric figures of merit at room temperature of about 1 could be attained, which is two orders of magnitude larger than that of bulk single crystals. However, although low dimensionality is effective at enhancing thermoelectric efficiency, it unavoidably decreases the device heat acceptance, as a large amount of the available heat flux is shunted through the NW template. Thus, higher efficiencies are paid in terms of lower heat fluxes being converted – leading to small electric power densities.

To avoid such shortcomings, we have developed a wet-chemistry approach based on one-pot Metal-assisted Chemical Etching (MaCE) that let fabricate dense, unsupported arrays of Si nanopillars, namely Si NWs aligned normally to the substrate. In our implementation, one-pot MaCE uses hydrofluoric solutions wherein a silver salt is dissolved. Silver ions act at one time as oxidant and, when reduced to metallic silver, as electrocatalyst, localizing the etch process and ultimately leading to the formation of Si nanostructures. Further to its simplicity and scalability, the technique displays a notable flexibility and could be used to obtain quite different classes of thermoelectric devices.

First, MaCE was used to obtain arrays that could be used as thermoelectric generators (TEGs) with heat flowing normal to the substrate. TEGs were found capable of large output power densities (up to 1 W/m2) even over small (20 K) temperature differences.

MaCE could also be used to obtain Si ‘nanofelts’, namely intertwined, self-supported nets of Si NWs providing pellet-like thermoelectric legs with thicknesses of some millimeters, yet with the low k of Si NWs. Thus, nanofelts let manufacture generators with the standard TEG layout, thus further moving NWs to the macroscale, which is needed by TEGs to provide significant power densities.

Finally, arrays of Si nanopillars grown on Si thin films by MaCE could be used to obtain nanostructures wherein Si nanopillars act as phonon resonators. Localized NW phonon modes are injected into bulk silicon to reduce its k while preserving its electrical conductivity and thermopower.

In summary, MaCE has demonstrated to be a very flexible tool to obtain high-density Si nanostructures that will promote the use of silicon in thermoelectric generators, both integrated and bulk.

Abstract ID: 558

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Optical properties and spectroscopy of graphene and other two-dimensional materials

Keywords: Perovskites, Quantum Dots, Magic Sized Clusters

Novel Properties of Metal Halide Perovskites: From Molecular Clusters to Magic Sized Clusters and Quantum Dots

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Metal halide perovskites (MHPs) with ABX3 (A for organic or inorganic cation such as Cs+ or CH3NH3+, B for metal cation such as Pb2+, and X- for halides-Cl, Br or I) structure exhibit novel electronic, optical and magnetic properties that have strong potential applications in emerging technologies including photovoltaics (PV) and light emitting diodes (LEDs). However, instability due to various factors presents a major challenge to their applications. The surface of the perovskites strongly affects stability. We have designed and demonstrated different surface passivation strategies to stabilize perovskite quantum dots (PQDs) and bulk films using surface chemistry approaches based on molecular ligands. One important finding is that ammonium ions and carboxylate groups have synergistic effects in surface passivation, attributed to simultaneous passivation of both anionic and cationic defects. Furthermore, we have recently found a simple strategy to synthesize and stabilize perovskite magic sized clusters (PMSCs), including doped PMSCs, for the first time, that exhibit interesting optical properties important for emerging applications such as single photon emitters. In our effort to understand the growth mechanism of PMSCs, we discovered a new species that we call molecular cluster (MCs) that do not contain the A component of the perovskites. The MSCs can be converted into more stable MCs while under appropriate experimental conditions MCs can converted into MSCs. Our studies demonstrate that surface chemistry approaches are promising for stabilizing MHPs, leading to generation of PMSCs, QDs, and ultimately QD solids, which is significant for many emerging applications.

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Abstract ID: 559

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Hard and Soft Magnetic Materials

Keywords: Rare-earth free permanent magnets, nano-crystalline, Computational materials design

Applying Computational Materials Science to Crystalline and Nano-Crystalline Magnetic Materials Design

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COVID-19 pandemic is changing our social infrastructure faster than we realize and rapidly revolutionizing the transportation sector industry. The significantly changing sector we face is the goods delivery system in urban and suburban areas. The delivery system uses small gasoline trucks and electric drones for now and will eventually change them to autonomous, medium-powered electric trucks and drones with high-speed data transfer communication system such as 5G; and even 6G networks. Motor quality and cost primarily determine the electric truck and drone's performance and economy. The critical component and most expensive part of a truck or drone's motor are magnetic materials. Therefore, one needs to develop a rare-earth (RE) free, permanent magnet with high maximum energy product (BH)max and also nano-crystalline soft magnet with high magnetization, high electrical resistivity, and small magnetostriction. Computational materials science has a crucial role in the discovery or advancement of magnetic materials.

We will introduce computational materials design methods and present our recently studied RE-free permanent and nano-crystalline (amorphous) soft magnets. Future research work on magnetic materials will be suggested.

Abstract ID: 560

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanomaterials and Nanotechnology

Keywords: Ionic Liquids, Colloidal Systems, Nanoreactors, Advanced Materials

Ionic Liquids Based Colloidal Solutions as Nanoreactors for Advanced Materials

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Room temperature ionic liquids (RTILs) are the organic analogues of inorganic molten salts with melting temperature <100oC [1]. Being ionic in nature, these compounds are versatile in terms of solvent properties such as low volatility, high thermal stability, wide liquid range and good solvating ability. In view of flexibility of choice of cations or anions, RTILs can designed as low viscosity media suitable for self-assembling of amphiphile molecules or also can also be designed as surfactants by incorporating amphiphilic character in either cation or anion or in both the constituents. Therefore, with extraordinary properties it has been possible to include RTILs as media or as surfactant or both for preparation of colloidal formulations/self-assembled structures [2]. Such structures are highly thermally stable and can be used as recyclable templates for preparation of shape/size controlled nanomaterials/quantum dots/metal organic frame works (MOFs), carbon dots (CDs) and hybrid materials [3,4]. We have constructed a stable ionic liquid colloidal system, where low viscosity ethyl ammonium formate IL is used as medium, R (+) limonene as non-polar medium, and bio-based surface active Choline[AOT] as an amphiphile. Self-assembled structures, thus constructed, have been utilized as recyclable nanoreactors for synthesis of a variety of shape and size controlled MOFs viz. HKUST-1, Uio-66-NH2, ZIF-8, and MIL-53(Al)-NH2 at room temperature in a generalized approach. The synthesized MOFs have been studied for gas adsorption and preparation of composite membranes for mixed salt separation applications.

Abstract ID: 561
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Recycling and sustainability of composite materials
Keywords: PWT, TAC, Adsorption, Heavy metals removal.

Using Pulverized Waste Tire and its Activated Carbon as Adsorptive Fill Materials

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In this study, the potential of pulverized waste tires (PWTs), either on their own or derived as activated carbon, to act as adsorptive fill materials was evaluated by conducting laboratory tests for accessing their adsorption and geotechnical properties. PWT (0, 5, 10, 15, 25, and 100 wt%) was mixed with soil to evaluate the removal of BTEX components and two heavy metal ions (Pb2+ and Cu2+). Also, the efficiency of tire- derived activated carbon (TAC) using carbonization and chemical activation techniques was assessed for removal of three synthetic heavy metal ions (Pb2+, Cu2+ and Zn2+). The results showed as the PWT portion increased, the adsorption of BTEX was also increased. Among the mixtures, the pure PWT showed the highest adsorption capacity toward the BTEX removal with the uptake capacity for xylene, ethylbenzene, toluene and benzene were 526, 376.9, 206.6 and 126.8 µg·g-1 of sorbent, respectively. TAC exhibited great potential to adsorb heavy metals, with monolayer adsorption capacities as high as 322.5, 185.2, and 71.9 mg·g−1 for Pb2+, Cu2+ and Zn2+, respectively, which were significantly higher than the adsorption capacities exhibited by commercial activated carbon (CAC), which were 42.5, 15.0, and 14.0 mg·g-1 for Pb2+, Cu2+ and Zn2+, respectively. Moreover, the obtained shear strength parameters for mixing tire and soil were at a favorable range, which showed that the mixture of tire and soil could be used as adsorptive fill materials.

Abstract ID: 562
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Polymeric composites
Keywords: PFOA, Chitosan, Adsorption, Amin functional group

Removal of Perfluorooctanic Acid (PFOA) from Aqueous Solution by Grafted Chitosan

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Perflurooctanic acid (PFOA) is environmentally persistent halogenated hydrocarbon, which has been widely used in many industrial and commercial applications. Recently, contaminating the soil and groundwater due to ubiquity of PFOA in environments has raised great concern. Adsorption technology is one of the most promising method for PFOA removal. Chitosan is a biopolymer substance with abundant amine and hydroxyl functional groups, which render it as a good adsorbent. This study, has tried to enhance the adsorption capacity of chitosan by grafting more amine functional groups on its surface. Series of batch adsorption tests have been performed to evaluate the adsorption capacity of the modified chitosan. Also, the raw and modified chitosan were analyzed by SEM, FT-IR, zeta potential, and XRD tests. The results demonstrated the aminated chitosan has good potential for adsorbing PFOA from aqueous phase because of its electrostatic interaction potential.

Abstract ID: 563

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Fiber reinforced Composites

Keywords: Glass Fiber Reinforced Polymer (GFRP), Epoxy resin, Fracture energy

GFRP Full Adhesive Connections: Mechanical Aspects

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In the field of the fiber reinforced polymer materials the efficiency of the adhesive technique versus the classical ones, bolting and welding, has been demonstrated by several studies available in the literature [1,2]. The main advantage of adhesive technique is relative to the absence of holes, then the stresses are more uniformly distributed over the bonded surfaces and stress concentration and damage to the fibers caused by the holes are non-existent. Furthermore, the stiffness and strength of adhesive joints is generally sensibly higher than those of bolted connections [3]. On the contrary, full adhesive joints present a brittle unsolicited behavior as well as an innate absence of plasticity limiting the diffusion on this technique in the field of civil engineering in particular. Within this framework several studies were developed to the study of hybrid connection (bonded and bolted at the same time), using the stiffness of the adhesive and the plasticity of steel bolts [4-5]. The main conclusion of these studies is that the strength of the hybrid connection is strictly function of the adhesive layer while the steel bolts represent a plastic reserve.

Relative to the field of full adhesive connection between FRPs members, in the present paper a wide experimental study is presented concerning the study of the mechanical response of a beam-to-column connection. Several parameters were taken into account: the extension of the adhesive surface, the load condition (shear and shear with bending) and the contribution of the GFRP angles. The test set-up was equipped not only with several displacement transducers in order to evaluate the load-displacement and moment-rotation curves but with the Digital Image Correlation system also. The latter allowed to understand the strain/stress distribution inside the adhesive layers giving the possibility to govern the strength and stiffness of the beam-to-column connection in function of the mode II of fracture energy being the only fracture energy considered. Furthermore, two different levels of fracture energy were taken into account: the total fracture energy, corresponding to the complete collapse of the joint; and the fracture energy level corresponding only to the linear behaviour of the connection.

Abstract ID: 564

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Photonic devices and applications

Keywords: microcavity lattice, structural defects, quantum dots, polaritonic excitations, virtual crystal approximation

Polaritonic nonideal supercrystals formed by 1D and 2D arrays of microcavities containing ensembles of quantum dots

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Designing and utilization of novel materials for manufacturing of the sources of coherent irradiation is currently a vast interdisciplinary area, which spans various theoretical and fundamental aspects of laser physics, condensed matter physics, nanotechnology, chemistry as well information science. Physical realization of corresponding devices requires the ability to manipulate the group velocity of propagation of electromagnetic pulses, which is accomplished by the use of the so-called polaritonic crystals. The latter represent a particular type of photonic crystals featured by a strong coupling between quantum excitations in a medium (excitons) and optical fields.

We considered 1D and 2D polaritonic crystals as a topologically ordered systems – arrays of coupled microcavities containing quantum dots. It is of substantial interest to investigate electromagnetic excitations in a non-ideal one-dimensional microcavity lattice subjected to a uniform elastic stress. The one-sublattice array of identical cavities contains randomly embedded quantum dots of two types. Moreover, these microcavity-resonators are also randomly removed at distances between the nearest neighbors. In order to calculate [1] polaritonic spectrum of such a system we shall adopt the virtual crystal approximation, which is based on diagonalization of the averaged Hamiltonian. The peculiarities of polariton spectrum in the 1D and 2D lattices of microcavities caused by the presence of the structure defects and uniform elastic deformation of the micropores array with quantum dots are studied. The presence of deformation and of structural defects may lead to an increase of the effective mass of corresponding excitations and therefore to a decrease of their group velocity. The results of numerical calculation performed on the basis of the constructed model contribute to modeling of the new class of functional materials – photonic crystalline system constituted of couple microcavities.

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Abstract ID: 565

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Ferroelectricity and piezoelectricity

Keywords: Layered ferroelectric ceramics, Molten salt synthesis route, Dielectric properties

Materials processes and characterization of rare earth doped layered ferroelectric ceramics for random access memory devices

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Modern computer systems employ the nonvolatile random access memory (NVRAM) device embedded in an integrated chip to store information. Ferroelectric random access memory has been utilized in NVRAM owing to its distinct properties such as low power consumption; fast read/write performance and high endurance compared to other electrically driven memory devices. Even though the classical ferroelectric lead zirconate titanate material has been extensively studied, practical application of this material is limited since it undergoes severe polarization fatigue during cyclic polarization switching and also this material is highly toxic. On the other hand, the renewed interest stems from the layered ferroelectric materials such as SrBi2Ta2O9, SrBi2Nb2O9, BaBi2Nb2O9, Bi4Ti3O12 due to the low fatigue with polarization switching and nontoxicity. However, these materials exhibit two significant drawbacks: High processing temperature and low remnant polarization. It is recently found that trivalent rare-earth ions doping on the crystal lattice of these layered ferroelectric materials significantly influence the physical properties. In our present research, the influence of samarium ion doping on the structural, microstructural, dielectric and electrical conductivity characteristics of SrBi2Ta2O9 and BaBi2Nb2O9 ferroelectric ceramics synthesized by molten salt synthesis route has been investigated in detail. The X-ray powder diffraction studies have revealed monophasic perovskite crystalline structure of different concentrations of samarium ion doped ferroelectric ceramics. The existence of plate-shaped morphological features of these ceramics has been demonstrated through scanning electron microscopic studies. The dielectric and electrical conductivity characteristics on these ceramics have given unique insights into the structural - property correlations. This talk shall provide a brief overview of layered ferroelectric materials widely employed in random access memory devices and present our recent research on the influence of rare-earth ion doping on their physical properties.

Abstract ID: 566
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Dielectric, Ferroelectric and Piezoelectric materials
Keywords: Ferroelectric, Negative Capacitance, Epitaxy

About negative capacitance in ferroelectrics

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The negative capacitance effect (NC), thought to be present in ferroelectrics, was suggested as a possible solution to overpass the Boltzmann tyranny, stating that the swing factor (S) between the OFF and ON states of a field effect transistor cannot be lower than 60 mV/decade. Many studies were devoted to investigate the nature of NC, and there are also many reports claiming values of S well below the one fixed by thermodynamic considerations. However, there is a string debate if NC is only a transitory effect or is a static one. In this contribution we bring evidences that NC is a transitory effect, closely related to polarization switching and to a fall of the ferroelectric resistance of about two orders of magnitude in epitaxial layers. Correlated electrical and piezo-force microscopy (PFM) investigation suggest that, in some cases, the switching takes place without formation of domains with opposite directions of polarization.1 A new method was developed, named the dynamic dielectric characterization, allowing to estimate the values of the elements of a ferroelectric capacitor from the current response recorded while a trapezoidal voltage pulse is applied on the sample.2 Further on, the relation between NC and structural quality of the ferroelectric film and its density of charge carriers is investigated. It is found that the NC effect fades in polycrystalline films, with complicated domain configuration and with reduced density of free carriers.

Key Words: Ferroelectric; Negative Capacitance; Epitaxy

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Abstract ID: 568
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Multifunctional composites
Keywords: Natural fibers, composites, impact, Amazonia

Natural fibers used from Colombia and their use as potential reinforcement for composite materials

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This investigation present results about the use of several natural fibers used in Colombia for centuries by ancient communities as cultural materials, some from the Andes mountains and others from the Amazonia region. Research present not only the traditional use, but also their potential use as reinforcement in natural composite materials. These fibers have been poorly explored from the engineering point of view. Indigenous and farmers have been using these fibers for millenniums as part of weapons, food preparation, ornaments, bags, and cultural uses. These natural materials and their composites were studied with scanning electron microscopy, X-ray diffraction, impact and other performance tests.

Abstract ID: 569

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrode/electrolyte interface phenomena

Keywords: Key Words: electrical double layer, near-electrode effects, near-electrode tomography, medium viscosity and dielectric constant, EC-AFM

Combined use of the EC-AFM in the near-electrode region. Comparison of "molecular" and "collective" effects*

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An approach to the investigation of the electrode-solution interfacial region is proposed, consisting in a combined study of the (I) molecular reactivity and (II) the properties of the medium, with the gradual displacement, increase in the distance L, from the electrode surface into the bulk. The first is carried out by a comparative structural analysis of the products of direct electrolysis vs. homogeneous electro-catalysis, for specially chosen substrates, under gradual increase in the L (the method called "near-electrode tomography", NELTO). The second, in addition to the classical methods of studying the electrical double layer, involves measurements of the viscosity, of the dielectric constant, etc., using electrochemical atomic force micro-scope EC- AFM -techniques.

By comparing the data of the NELTO on changes in „molecular effects" x = f(L)

with the changes in "collective effects" X =F(L), the new possibilities arise for esta-blishing the nature of phenomena in the interfacial area. Along with the effects of re-activity, the data of spectral structural nano-measurements can be used as 'molecular'. Some results are given and details of this approach are discussed.

Key Words: electrical double layer; homogeneous electro-catalysis; near-electrode effects; near-electrode tomography; medium viscosity, dielectric constant; tribology; EC-AFM

*Presented in part in [1]

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Abstract ID: 570

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Ceramic based composites

Keywords: Thermoelectric oxides, Solar Sintering, rGO nano-composite, SrTiO3

Improving the thermoelectric properties of solar sintered Nb-doped SrTiO3 with addition of reduced graphene oxide

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Over the last decade, there has been growing interest in the development of high-temperature thermoelectric (TE) oxides for the automotive and energy-harvesting sectors. The interest in oxide TE is due to their low toxicity, low cost and high chemical robustness. Recent reviews have highlighted the potential of a range of oxides including those based on SrTiO3 (STO), ZnO, TiO2, CaMnO3and Ca3Co4O9. Of these materials, STO has attracted tremendous interest as an n-type TE oxide for its large carrier effective mass, stability at high temperature and structural tolerance with respect to doping. The electrical conductivity in STO can be achieved by donor doping with higher valence ions especially in the Ti-site and by reduction to generate oxygen vacancies. Similarly, graphene-derived materials have attracted much attention and their composite with oxides have also a wide application in conductive switching or photocatalysis. However, the application of graphene or rGO in oxide-based TE materials is limited to undoped STO, La-doped ST, and recently reported Nb-doped STO.

To achieve optimum density in oxide materials for TE applications, a minimum sintering temperature of 1400oC is essential. Achieving such high temperatures in electrical furnaces is energy-intensive, exploiting electric energy generated from non-renewable energy resources which have substantial financial and environmental impact related to the high thermal budget and Green House Gas (GHG) emissions, respectively. On the other hand, concentrated solar energy, with the capability of converting concentrated solar radiation into high-temperature heat, has proved to have valuable and reliable results in a lot of applications such as electricity generation, production of hydrogen and solar fuels, water treatment, heating systems and research in advanced materials.

In this work, Sr (Ti0.90, Nb0.10)O3 prepared by conventional solid-state reaction technique were mixed with 5 wt% and 10wt% of graphene oxide (GO) prepared by Hummer-based method. The composite mixtures were sintered in a solar furnace in H2/N2 atmosphere to reduce both Nb-doped SrTiO3 and GO. It is observed that the ZT value of Nb-doped SrTiO3 was enhanced multi-fold by rGO nano-inclusions. The addition of reduced GO enhanced the electrical conductivity, σ, while suppressing the thermal conductivity, κ. These findings provide useful enlightenment on enhancing the thermoelectric properties in Nb-doped STO by nano inclusions of rGO and offer further prospects for developing high-performance oxide thermoelectric materials for energy harvesting.

Abstract ID: 571

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Fuel Cells

Keywords: fuel cells, ink, ionomer, limiting current, catalyst layer

Structure from Darkness: Exploring Ionomer interactions in Fuel-Cell Inks and Resultant Performance Impacts

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The fabrication of proton-exchange-membrane fuel-cell catalyst layers is traditionally an empirically based black art. These layers are typically fabricated from multicomponent inks composed of Pt/C nanoparticles, a dispersion of ion-conducting polymer or ionomer, and all in an alcohol/water mixed solvent system. These inks are then coated onto ionomer membrane or gas-diffusion layers using different techniques such as ultrasonic spray and then allowed to dry to form a triple percolated pathway for gas, ions, and electrons to transport and react at the catalyst sites. Thus, the interactions within the ink control the catalyst-layer structure and resultant performance. In this talk, we will explore the underlying interactions of the constitutive components of the fuel-cell inks, with a focus on how the ionomer and catalyst interact. Such studies include isothermal titration calorimetry, dynamic light scattering, zeta potential measurements, and quartz crystal microbalance. These studies will be complemented by in-situ characterization of fuel-cell performance and limiting current analysis for different ionomers. The findings demonstrate the key roles that ionomer content and identity play in interacting though hydrophobic forces with the particle surface and controlling catalyst-layer structure and performance. It will be shown that higher ion-exchange polymers result in larger interfacial interactions but lower local transport resistances. The studies provide insights into catalyst-layer fabrication and point to future material design trends and targets for these functional composite materials.

Abstract ID: 572

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Fuel Cells

Keywords: Fuel Cell Membrane, Polymer Electrolyte, Polyacrylonitrile, acid-doped membrane, Ion Exchange

Synthesis and Characterization of Polyacrylonitrile (PAN) Nanocomposite for Proton Exchange Membrane Materials in Fuel Cells

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Fuel cells (FCs) is the future potential promising candidate for a power source providing a renewable and clean energy for remote power supplies, portable power devices, stationary power generations, and a wide range of transportation applications (1). The membrane is one of the essential components in proton exchange membrane (PEM) fuel cells (2). Membranes should be high thermal stability, high protonic conductivity, low electronic conductivity, good mechanical properties to ensure the achievement of the fuel cell (3). Therefore reliability, stability and durability of the membranes used for PEM fuel cells are still under continuous assessments.

In this study, phosphoric acid doped polyacrylonitrile (PAN) nanocomposite membranes were prepared by dispersion of various amounts of fumed silica particles and borax decahydrate in PAN polymer matrix followed by phosphoric acid doping as the proton conducting agent. Electrochemical Impedance Spectroscopy (EIS), TGA, XRD, FTIR and SEM were used to characterize membrane samples produced by using electrospinning technique and solvent casting method. The results showed that the membranes have high performance relative to commercially available Nafion membrane.

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Abstract ID: 573

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Ferroelectricity and piezoelectricity

Keywords: Ferroelectric Domains, (K, Na)NbO3 Epitaxial Film, X-Ray Diffraction, Phase-Field Simulations

Ferroelectric Phase Transitions in Strained K0.9Na0.1NbO3 Epitaxial Films Studied by in situ X-Ray Diffraction and Three-Dimensional Phase-Field Simulations

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A high-temperature phase transition in strained ferroelectric K0.9Na0.1NbO3 thin films epitaxially grown on orthorhombic (110) NdScO3 substrates is identified and investigated both experimentally by three-dimensional in situ X-ray diffraction and theoretically by three-dimensional phase-field simulations. At room temperature, the thin films show a strongly anisotropic misfit strain that induces the appearance of monoclinic a1a2/MC phases. This phase coexistence leads to the formation of a regular, herringbone domain pattern. With increasing temperature, a ferroelectric-to-ferroelectric phase transition to an orthorhombic a1/a2 phase takes place. This is accompanied by a regular stripe domain pattern with exclusively lateral electric polarization. Corresponding simulations of the scattered X-ray intensity patterns show that the orthorhombic unit cells exhibit a small in-plane rotation. This leads to four different in-plane orientations of the orthorhombic unit cells and, correspondingly, to four variants of superdomains. The experimental results are fully consistent with three-dimensional phase-field simulations using anisotropic misfit strains. This applies in particular to (i) the three-dimensional domain wall arrangement in room and high-temperature phases and (ii) the broad phase transition range between about 180 °C and 260 °C, where a complex interplay of coexisting monoclinic a1a2/MC and orthorhombic a1/a2 phases occurs [1,2].

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Abstract ID: 574
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Nanocomposites
Keywords: PMMA, Nano, Optical constant, Hot-Probe, Titanium dioxide.

Evaluation of impurities concentration with hot probe method and optical constants of nanostructured titanium dioxide embedded polymer thin films

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Electrical and optical characteristics of nano particle embedded polymer thin films significantly differ from those of pure polymers. Therefore, characterization methods for evaluation of nano particle embedded polymer thin film became highly important. A novel approach to the well-known “Hot-Probe” method is applied in present work. The conventional Hot Probe characterization method enables the definition of a semiconductor type, P or N, by identifying the majority charged carriers. According to the Hot Probe technique, one can measure and calculate the majority charged carriers concentration and its dynamic parameters. In the present report evaluation of majority charged carriers concentration of nano sized titanium dioxide embedded PMMA polymer is carried out with Hot Probe technique. The polymer samples are prepared with various concentration of nano sized titanium oxide using casting method. Optical constants of these samples are also determined using transmission and reflection curves in wide range of wavelengths.

Abstract ID: 575

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Phase Change Materials

Keywords: Light-induced phase transitions, Optical Properties, Phase-change materials

Light-controlled stepwise (multilevel) changing properties of chalcogenide-based thin films as promising materials for photonics and optoelectronics application.

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Thin film chalcogenide materials such the GeTe, GeSbTe, GeSbSeTe are widely used in photonic, optoelectronic devices, since their physical properties differ significantly for two stable phase states – crystalline and amorphous [1]. In this work we observed a multilevel reversable changing in optical properties of thin film samples, related on the light-induced phase transitions under impact of nanosecond pulsed laser radiation. Device based on chalcogenide thin film is able to be programmed into multiple states that correspond to different amorphous/crystalline phase ratio [2, 3]. The high optical contrast in the spectral range from 200 nm to 22000 nm and high difference in electrical conductivity between amorphous and crystalline states was demonstrated early [4]. The switching between multiple states was controlled by pulsed radiation of the 532 nm 20 ns laser with differs of energy flux in pump-probe scheme realised by us in [5]. Numerical model based on heat transfer in solids and classical Stefan problem was used to predict the ratio of amorphous/crystalline phase states. This study offers a promising way of creation of new devices based on chalcogenide thin films, such a multilevel phase change memory and optical neuromorphic systems.

Key Words: Light-induced phase transitions, Optical Properties, Phase-change materials

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Abstract ID: 576

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Bio-inspired design of composites

Keywords: Biosilica; Nanoparticles; Nanostructures; Microbioreactors

Bio-factory mediated and biomimetic approaches for the synthesis of SiO2- based nanostructures for multiple applications.

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A novel biotechnological approach to the preparation of Ir-doped luminescent silica-based nanostructures is proposed availing use of diatoms microalgae which generate highly nanostructured biosilica shells (frustules) by in vivo biomineralization of orthosilicic acid [1]. After the in vivo incorporation of a phosphorescent organometallic complex (Ir-1) in Thalassiosira weissflogii diatom frustules (DFs), bulk functionalized phosphorescent silica-based nanostructures are obtained by isolation and proper ultrafine processing of Ir-1-doped DFs. High-resolution characterization reveals the presence of phosphorescent hybrid organic/inorganic clusters composed of biogenic silica NPs intimately trapped within the diatom organic residual matter. The biofactory strategy investigated herein can be a sustainable, cost-effective, and scalable route to transition metal-doped silica nanomaterials and can pave the way to a great variety of heavy-metal and rare-earth metal doped silica nanostructures, whose applications range from photonics to imaging, sensing, and biomedicine.

Inspired by the biosilica morphogenesis, which takes place inside the diatom cell within the silica deposition vescicle (SDV), a specialized membrane-bound compartment, we set up a biomimetic/bioinspired design and synthesis of structural and functional hybrid organic/inorganic SiO2-based nanostructures (NSs), which present many distinctive advantages over traditional chemical synthesis methods. The intriguing ability of diatom long chain polyamines (LCPAs) to rapidly induce precipitation of SiO2 spheres has motivated the in vitro one-pot synthesis of SiO2 particles. Therefore, the templating by amine-bearing molecules is seen as a successful biomimetic approach for the synthesis of SiO2-based hybrids under mild and environmentally friendly conditions for biosensing and biomedical applications. [2].

Key Words:Biosilica; Nanoparticles; Nanostructures; Microbioreactors

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Abstract ID: 577
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Ceramic based composites
Keywords: Additive, Preceramic, Packaging

Additive Manufacturing of Polymer-Derived Ceramic Composites

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Reinforcement of ceramics with a second ceramic phase is a well-established method to create a composite with strength and toughness beyond either constituent material. However, 3D printing approaches that rely on surface interactions for sintering are limited in the amount of reinforcement that can be incorporated. Here we discuss the addition of ceramic reinforcement media to silicon-based, pre-ceramic resins that can be printed on commercial stereolithography printers and subsequently converted into a ceramic matrix composite (CMC) by pyrolysis [1]. We will discuss the use of various reinforcement materials, form factors (e.g. particles and whiskers) and volume fractions in relation to performance and compatibility with the printing method. The CMCs are over an order magnitude stronger and four times tougher than the base polymer-derived ceramic [2]. In addition, we investigate the high temperature (>1000C) properties of the 3D printed CMCs. Recently we have applied this technology to fabrication of complex packaging for 3D integration of microelectronic subsystems and initial results will be presented

Key Words: Additive, Preceramic, Packaging

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Abstract ID: 579
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Composite structural materials
Keywords: Temperature dependence, Strength, Hardness, Elastic modulus

Temperature dependence of the physical and mechanical characteristics of borides and metal multielement alloys

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The theoretical strength, Young's modulus and their temperature dependence are calculated using the pseudopotential method taking into account the quasi-harmonic approximation and presented in analytical form.

Unlike the moduli of elasticity and theoretical strength, hardness has no theoretical analogy. When calculating hardness, experimental information is used as a fitting parameter. Based on the phenomenological theory and taking into account that we are interested in the temperature dependence of mechanical properties, the hardness of the crystal is presented as a function of the lattice parameter and an adjustable parameter, which depend on temperature.

An analytical formula is derived from first principles that describes the temperature dependence of the lattice parameter for metals, multielement metal alloys, transition metal borides, and also quasi-binary boride eutectic systems. For multi-element alloys, a model has been developed to take into account solid solution hardening.

To take into account the temperature dependence of the adjustable parameter, it is proposed to use the limiting condition: at the maximum temperature, the hardness disappears (in contrast to the characteristics of elasticity or strength). As a result, the temperature dependence of the mechanical characteristics was obtained.

Using the presented ratios, it is possible to estimate the elastic modulus, theoretical strength, hardness of multi-element metal alloys and borides at any temperature in the presence of their melting points and the listed characteristics at zero temperature (strength, Young's modulus, hardness).

Abstract ID: 580

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: All solid-state batteries

Keywords: Solid-State batteries, Li metal, Interfaces, Dislocations, Composite, Energy Storage

Interfaces in Solid-State Li Batteries

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Despite all the progress made in the development of solid-state Li batteries (SSLB), interfaces arise as the main bottleneck impeding their practical realization. In particular, the interfacial regions between the individual components of a cell comprising those formed between ceramic electrolytes and Li metal and ceramic high-voltage cathodes as well as interfaces between ceramic particles and the polymeric matrix in composite electrolytes are identified to be challenging.1 For example, current constriction that arise from inhomogeneous electrical field distributions at the Li metal | solid-electrolyte interface leads to the formation of dendritic structures at high current rates.2 Forming a good interface between the solid electrolyte and cathode material requires high temperature treatments that leads to the formation of an interphase layer that impedes the ion transport across the interface.3 To unroll the beneficial properties of a composite membrane both components, ceramic particles and polymer matrix, must contribute to the long-range ion transport. Due to the high interface resistance between the components, ionic transport does not take place in ceramic particles; hence, the ceramic has only the role of a passive filler rather than improving the membrane properties.4

Inspired by these challenges, mitigation strategies to overcome these bottlenecks will be presented. For example, strategies that (i) enable cycling at very high rates up to 6 mA cm-2 using different surface treatments and current waveforms, (ii) change the mechanical properties at the interface to potentially avoid crack formation that ultimately leads to short circuits, and (iii) lower the interfacial resistance between ceramics and polymers by orders of magnitude.5 Moreover, we show that Co interdiffusion not only lead to the formation of resistive interphases, but is also detrimental for the electrical transport properties and electrochemical stability of solid electrolytes.

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Abstract ID: 581

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Optical properties of metals and non-metals

Keywords: Ag-AgCl thin film, Waveguide, Plasmonic nanostructure

The effect of higher-order TE modes in AgCl waveguide on optical and structural properties of plasmonic nanostructures

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Silver chloride (AgCl) thin films loaded by silver nanoparticles (AgNPs) are nanoscale plasmonic materials, which can storage the polarization and wavelength of incident light beam in the whole range of visible light spectrum. The AgCl thin film is a sub-wavelength waveguide, that its thickness determines the cutoff frequency and the number of modes which can propagate in this thin film. The AgNPs on the surface of AgCl thin films scatter the incident polarized beam and then a part on the incident beam traps in the AgCl waveguide. The superposition of each propagated mode in AgCl waveguide with incident light beam, creates an interference pattern on the surface of AgCl thin. The AgNPs aggregate in the dark fringes of interference pattern and form an ordered plasmonic nanostructure in direction of light polarization on the surface of AgCl thin film. The ordered plasmonic nanostructures not only contain information about incident light beam, but they also carry information about the propagating modes in waveguide and refractive index of substrate. We fabricate AgCl thin film with three different thicknesses to investigate the effect of TE0, TE1, TE2 modes on the optical and structural properties of plasmonic nanostructures create on the surface of AgCl thin film.

Abstract ID: 582
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Smart Composites
Keywords: PMMA-silica hybrid, anticorrosive coating, self-healing, cerium, lithium

Lifetime improvement of anticorrosive hybrid coatings by addition Li and Ce self-healing agents

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Organic-inorganic coatings based on polymethyl methacrylate (PMMA)-silica hybrids provide effective and active corrosion protection of metallic surfaces against corrosive species. The covalent conjugation on the molecular scale between and the PMMA matrix, provided by the propyltrimethoxysilane or 2-hydroxyethyl methacrylate coupling agent, leads to a homogenous and highly cross-linked nanocomposite, which in form of coatings act as an efficient diffusion barrier. Transmission electron microscopy, small-angle X-ray scattering, and thermal analysis data showed that the addition of increasing amounts of lithium carbonate or cerium ammonium nitrate (0, 500, 1000, 2000, and 5000 ppm) to the silica precursor solution (tetraethoxysilane - TEOS) yields PMMA-silica coatings with increased connectivity of the silica cross-link nodes, uniformly distributed in a highly polymerized PMMA matrix. Results of electrochemical impedance spectroscopy (EIS) assays of coated aluminum AA7075 aluminum alloy, performed in a 3.5% NaCl solution, showed that the addition of Li or Ce provides for both coating systems the self-healing ability resulting in a significantly improved lifetime up to 720 days and an impedance modulus of up to 50 GΩ cm2. Time-of-flight secondary ion mass spectrometry, scanning electron microscopy and X-ray photoelectron spectroscopy suggest that the regeneration process occurs by leaching of lithium/cerium ions from the coating surface into the corroded area, which is restored by a protective layer of precipitated species.1 An analog mechanism was found for artificially scratched coatings presenting an impedance modulus increase after neutral salt spray test compared to the bare aluminum alloy. These findings evidence the active role of lithium and cerium ions in improving the structural properties of hybrid coatings and providing through the self-healing ability a significantly extended service time of metallic components.

Abstract ID: 583

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Electrode/electrolyte interface phenomena

Keywords: operando soft x-ray spectroscopy, electrochemical interface, Li-ion/Mg-ion batteries, catalysts

Operando soft x-ray spectroscopy for interfacial characterization of energy-storage materials and chemical transformation

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The energy materials and devices have been largely limited in a framework of thermodynamic and kinetic concepts or atomic and nanoscale. Advanced energy technology arises from the understanding in fundamental science, thus rest in large on in-situ/operando characterization tools for observing the physical and chemical interfacial processes. Synchrotron based x-ray spectroscopic techniques offers unique characterization in many important energy materials of energy conversion, energy storage and catalysis in regards to the functionality, complexity of material architecture, chemistry and interactions among constituents within.

In the operando soft x-ray spectroscopy characterization of interfacial phenomena in energy materials and devices, it has been found that the microstructure and composition of materials as well as the microstructure evolution process have a great influence on performances in a variety of fields, e.g., energy conversion and energy storage materials, chemical and catalytic processes. However, it is challenging to reveal the real mechanism of the chemical processes. In-situ/operando x-ray spectra characterization technique offers an opportunity to uncover the phase conversion, chemical and environmental change of elements and other very important information of solid/gas and solid/liquid interfaces in real time.

It has been demonstrated how to best use the in-situ/operando soft x-ray spectroscopy characterization techniques, including soft x-ray absorption spectroscopy (XAS) and resonant inelastic soft x-ray scattering (RIXS) to investigate the real electrochemical mechanism during the operation. The experimental results show that in-situ/operando soft x-ray spectra characterization techniques can further enhance the understanding of real reaction mechanism.

Abstract ID: 584

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster/Oral Presentation

Topics: Solar Cells

Keywords: hick film screen printing, chemical replacement reaction, Al, Cu, Ag, conductivity, p-type bifacial PERC solar cell

Improvements in the efficiency of p-type bifacial Si solar cells with Cu electrode using galvanic replacement reactions

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Abstract

A novel method for fabricating the base metal Cu in an air atmosphere was successfully developed based on thick film screen printing of Al pastes and galvanic replacement reactions. The first thick film screen printed Cu electrode with high conductivity (<10-6 Ω-cm), which is comparable to thick film Ag electrode, was successfully made in air firing instead of reducing atmosphere firing.

In this study, we introduce high-efficiency p-type bifacial PERC solar cells with an industrial typical PERC process flow used to apply a screen-printed aluminum finger grid on the rear side of an electrode instead of a full-area aluminum layer. A novel copper (Cu) technique is used to fabricate the Cu electrodes that are substituted for Al electrodes in p-type PERT c-Si solar cells. F.F. and efficiency of the p-PERT solar cell with the novel copper electrode can be remarkably improved. The maximum efficiency of the p-type bifacial single crystalline solar cells obtained with this process was 23% for the front Cu side and 20.7% for the rear Cu side illumination under standard testing conditions (STC). The ratio between front and rear side performance was over 90% for all of the solar cells.

Key Words: Thick film screen printing, chemical replacement reaction, Al, Cu, Ag, conductivity, p-type bifacial PERC solar cell

Abstract ID: 585

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster/Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: 2D, Molybdenum disulfide, Thin film transistors, Electrohydradynamic jet

Electrohydrodynamic jet printed patterning of MoS2 using solution process for thin-film transistors

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Molybdenum disulfide (MoS2) is one of the most studied layered TMDCs due to its excellent optical, electrochemical, and electrical properties. Many research groups have attempted to synthesize MoS2 with different methods to make good MoS2 quality. Mechanical exfoliation and chemical vapor deposition (CVD) have been used to prepare MoS2 thin layers. Nevertheless, CVD method demanded vacuum and sulfurization resulted in expensive MoS2 films. Our group developed a new CVD-free sol-gel solution process for making MoS2 atomic layers without sulfurization. Even though the fabrication of uniform 2H-MoS2 thin film on wafer scale could be possible with controlled atomic layers, the electrical property was poor for practical electrical devices.

No report has been published using jet printing technology from MoS2 precursor solution so far. Therefore, the goal of this research was to develop a new drop-on demand printing method for MoS2 atomic layers based on sol-gel synthesis method. In this paper, the precursor solution and process were modified and applied in an electrohydrodynamic (EHD) jet printing system which features drop-on-demanding printing with high uniformity. EHD jet printing with Taylor cone jet mode was utilized to obtain MoS2 pattern lines from (NH4) 2Mo4 based solution for the first time. Most importantly, we proved the uniqueness of printed MoS2 atomic layers with high uniformity from bottom-up synthesis after printing and simple thermal annealing. The EHD jet-printed MoS2 TFT shows a high current ratio of approximately 5.0×106, a good mobility of 19.4 cm2 V-1 s-1.

Abstract ID: 586

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Electrical properties of graphene, Mxenes and other two-dimensional materials

Keywords: Phase engineering, TMDs, Topological Insulator

Semiconductor to Topological Insulator Transition in Transition Metal Dichalcogenides Core-Shell Lateral Heterostructures

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Polymorphic phase transition is an important route for engineering the properties of two-dimensional materials. Heterostructure construction, on the other hand, not only allows the integration of different functionalities for device applications, but also enables the exploration of new physics arising from proximity coupling. Yet, implementing a design that incorporates the advantages of both remains underexplored. In light of integrating heterostructure formation and phase engineering in one step, we demonstrate a novel phase transition technique based on the construction of lateral (WSe2/SnSe2) core-shell architecture by molecular beam epitaxy. A semiconductor to topological insulator (TI) transition associated with the polymorphic change of WSe2 core is revealed by scanning tunneling microscopy/spectroscopy in conjunction with first-principles calculations. Since the proposed phase transition mechanism only fundamentally requires a van der Waals interacting substrate and sufficient core-shell lattice mismatch, the approach could be potentially versatile towards other transition metal dichalcogenides and vapor deposition methods.

Key Words: Phase engineering, TMDs, Topological Insulator

Reference:

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Abstract ID: 587

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Electrochemical Supercapacitors

Keywords: Electric Double Layer Capacitors, EIS, Quality Assurance

A Multi-Channel Fast Impedance Spectroscopy Instrument for the Quality Assurance of Electric Double Layer Capacitors

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Conventional experimental methods for testing the performance of Electric Double Layer Capacitors(ELDCs) include the measurement of capacitance through charge and discharge, measurement of Equivalent Series Resistance (ESR) and measurement of self-discharge and the Equivalent Circuit Model (ECM) by Electrochemical Impedance Spectroscopy (EIS). However, the methods are not suitable for the mass production line of EDLCs since they require long time for the test and several kinds of different instruments. EIS is an attractive method to evaluate the performance of EDLCs except that it takes a long time for a single test. In this paper a fast EIS instrument suitable for quality assurance for the mass production of EDLCs is proposed. In order to reduce the time for the test, a multi-sine sweeping method is used for the EIS test and the results are analyzed by extracting the parameters of the ECM to evaluate the performance of the EDLCs. The proposed instrument is developed to have multi-channel to further decrease the time for the test with an EDLC. It is also presented as to how the extracted parameter values of the ECM can be used to evaluate the performance of the supercapacitor.

Abstract ID: 588

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Liquid electrolytes, ionic liquids, polymer electrolytes
Keywords: Silicon, Nano, Molten salts, Energy-related applications

Electrochemical production of high-purity silicon in molten salts towards energy-related applications

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Crystalline silicon solar cells have dominated the photovoltaics (PV) market for the past several decades and are most likely to continue to be the primary technology for the PV industry in the future due to its abundant raw materials supply and non-toxicity. One of the long-standing challenges is the high-purity silicon production cost because of its complex and energy-intensive production processes. In addition, nanostructured silicon as electrode material also has great potential for energy storage applications. However, cost-effective production of high-purity silicon materials still remains a challenge. The molten salt electrochemical process provides a possible alternative route for the cost-effective production of silicon for various energy-related applications. In this work, we present the demonstration of electrochemical production of high-purity silicon materials with different morphologies in molten salts. Silicon materials with tunable morphologies, i.e., dense silicon films, silicon nanowires, silicon particles were produced in a controlled manner in molten salts, and the reaction mechanisms involving an in-situ dissolution-electrodeposition process were systematically investigated. This study offers a promising route to facilely produce silicon materials for various energy-related applications.

Abstract ID: 589

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Photonic devices and applications

Keywords: conjugated polymer PFO-co-PPV-MEHB; sub-nanoscond TRS, amplified spontaneous emission (ASE) spectra; green emitter

An Efficient Green Mirror-less laser from Conjugated Polymer (PFO-co-PPV-MEHB) in Solution

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The purpose of this work is to investigate the optical and mirror-less laser properties of conjugated polymer (CO) Poly[(9,9-dioctylfluorenyl-2,7-diyl)-co-(1,4-diphenylene-vinylene-2-methoxy-5-{2-ethylhexyloxy}-benzene)] also known as [(PFO-co-PPV-MEHB), ADS125GE], dissolved in many solvents. The absorption and fluorescence spectra have been measured at various concentrations in different solvents such as benzene and toluene. The amplified Spontaneous Emission (ASE) spectra peaked approximately at 509 nm of CO PFO-co- PPV-MEHB in different solvents have obtained at suitable concentrations and pump energies. The pump source was third harmonic of Nd: YAG laser (355 nm) in transverse mode. The relationship between input pumping energy and output energy for the samples in solutions has been studied. In addition, the photochemical stability of this CO as a laser material was examined. The Time Resolved Spectroscopy (TRS) studies with sub-nanosecond resolution has been performed for CO under various pumping energy. These results have provided understanding of the excited state dynamics of CO PFO-co-PPV-MEHB and have shown that this new CO is quite efficient in the green region under Amplified Spontaneous Emission (ASE) Mode.

Abstract ID: 590

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: CdSe/ZnS and Ag-In-S/ZnS Core/shell Quantum Dots, Porphyrins, Self-Assembly, Pathways of Photoluminescence Quenching, 3D Model of Nanoassemblies

Nanoassemblies Based on Semiconductor Quantum Dots and Porphyrins: Formation Principles, Interface Effects, Optical Properties and Exciton Relaxation Pathways

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Organic-inorganic nanoassemblies based on colloidal semiconductor quantum dots (QDs) of various types in combination with functionalized organic dye molecules are used as perspective nanostructures for possible applications in sensing, photovoltaics, and biomedicine. Because of high surface-to-volume ratio in QDs, the physical and chemical properties of their surface play a significant role in determining the overall QD properties as well as those of nanoassemblies based on them. Correspondingly, the analysis of surface and interface processes in QD-dye nanoassemblies is the necessary step upon development of hybrid nanomaterials for possible applications. The intention of our report is a comparative description of surface properties, structural dynamics and pathways of excitation energy relaxation processes in QD-Dye nanoassemblies of two types: i) TOPO-capped CdSe/ZnS QDs being attached via coordination interactions with tetra-pyridylporphyrins in toluene, and ii) Ag-In-S/ZnS core/shell QDs (AIS, AIS/ZnS) stabilized by glutathione (GSH) and coupled with 5,10,15,20-(tetra-N-methyl-4-pyridyl)porphyn molecules via Coulomb attraction in water. Our discussion of a realistic scenario of the interactions between dye molecules and ligand-stabilized QDs is based on spectral-kinetic measurements (absorption/emission, Raman, time-resolved spectroscopy) and a constructed quantum chemical atomistic 3D model. Based on the experimental and theoretical analysis of the results obtained for QD-Porphyrin nanoassemblies, we show how surface-mediated processes dictate the probability of several of the most interesting and potentially useful photophysical phenomena (energy transfer, electron tunnelling in the conditions of quantum confinement, formation of intra-gap states, etc.) Basic results of this study may be useful in the directed formation of new nanoscale organic-inorganic building blocks and offer significant advantages in a wide areas of applications.

This work was funded by Volkswagen Foundation (Project “New Functionalities of Semiconductor Nanocrystalsby Controllable Coupling to Molecules”), BSPSR program “Convergence–2020 3.03”, RFBR grant № 18-53-00035 (Russia-Belarus), as well as by the European Union under Grant Agreement 732482 (Bio4Comp -Parallel Network-Based Biocomputation) and Visiting Scholar Program of TU Chemnitz, Germany(E.Z.).

Abstract ID: 591

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Electromagnetic radiation

Keywords: Implanted Metal, Corrosion, Biosensor, Total Hip Arthroplasty, Electromagnetic Radiation

Novel Investigation of the Effects of Ambient Electromagnetic Radiation on the Corrosion of Implanted CoCrMo Metal

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Although total hip arthroplasty (THA) is considered to be the most successful orthopedic operation in restoring mobility and relieving pain, common metal based implants developed in the past decade suffer from severe inflammatory reactions of the surrounding tissue caused by the premature corrosion and degradation of the implant. A substantial amount of research has been dedicated to the investigation of mechanically driven fretting and crevice corrosion as the primary mechanism of implant failure. However, the exact mechanism by which hip implant breakdown occurs remains unknown, as current in vitro fretting and crevice corrosion studies have failed to completely replicate the corrosion characteristics of recovered implants. Here, we show that minor electric potential oscillations on a model hip implant replicate the corrosion of recovered, failed implants without the introduction of mechanical wear. We found in a controlled lab setting that small electrical oscillations can force electrochemical reactions within a simulated synovial fluid environment that have not been previously predicted.

This work specifically investigates the potential corrosion response of high frequency nonionizing electrical oscillation, on the same order as that caused by ambient electromagnetic radiation, on a common biocompatible ASTM F75 CoCrMo metal alloy. Each day, the human body is subjected to significant electromagnetic radiation from manmade sources, ranging from residential electrical power at 60 Hz to cell phone technologies at 1-30 GHz, with magnitudes from ~300 mV/m to greater than 5 V/m. Such electrical oscillation is shown to produce substantial surface modification, and metal ion release into solution. This is in direct contrast to samples shielded from electromagnetic radiation via faraday cage, which present no significant surface modification, nor substantial interaction within the test solution. In lab testing we have shown the replication of a calcium, phosphorous, chromium, oxygen complex on the surface of a CoCrMo metal alloy test specimens, matching the chemical composition of previously retrieved wear particles from failed patient prosthetics. Our results demonstrate that the electrical activity and ensuing electrochemical activity excites multiple corrosion failure modes: direct dissolution of the medically implantable alloy, leaching metal ions into the body, and surface deposition growth, forming the precursor of secondary wear particles.

We anticipate our findings to be the foundation for the future development and testing of electrochemically resistant implantable functional materials. This newly identified electrochemical corrosion phenomenon must be taken into consideration during the development of advanced functional materials for biosensing application, which must perform consistently in a highly electrolytic environment under constant bombardment of electromagnetic radiation from an ever evolving technological society.

Abstract ID: 592
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Particulate reinforced Composites
Keywords: nanocomposite thin film, atmospheric plasma, DBD, APPJ, electrochemical impedance spectroscopy, colloidal suspension, corrosion, carbon steel

Nanocomposite coatings based on graphene and siloxane polymers deposited by atmospheric pressure plasma. Application to corrosion protection of steel

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Nanocomposite coatings based on graphene and siloxane polymers

deposited by atmospheric pressure plasma. Application to corrosion

protection of steel

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Nanocomposite coatings based on graphene and siloxane polymers

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In the present talk, graphene-based nanocomposite thin films were developed for the first time by a non-equilibrium atmospheric plasma to improve the corrosion resistance properties of E24 carbon steel. The nanocomposite coatings were prepared by a dielectric barrier discharge using a nebulized colloidal suspension of graphene nanosheets (GNs) dispersed in hexamethyldisiloxane (HMDSO) used as the precursor for the polymer matrix. After obtaining a stable colloidal solution, it was nebulized into the plasma reactor to form a plasma polymer (pp) coating from HMDSO (ppHMDSO) in which GNs were incorporated (GN@ppHMDSO) on the mild steel substrate. The chemical structure of the hybrid coatings was characterized by X-ray photoelectronspectroscopy and Fourier transform infrared spectrometry. Raman spectra of GNs and GN@ppHMDSO coatings suggest the existence of charge transfer between the GNs and the HMDSO matrix. Furthermore, scanning electron microscopy confirms the synthesis of micro/nanocomposite with a fairly homogeneous dispersion of the GNs in the polymer matrix. The corrosion resistant properties of the nanocomposites hybrid coatings GN@ppHMDSO

deposited by a one-step atmospheric pressure plasma process were evaluated by electrochemical impedance spectroscopy(EIS) and show an improvement of the corrosion protection effect, with an increase under optimal conditions(1 wt%. Fig 1A &B) of up to 3 orders of magnitude in the resistance to charge transfer on treated steel, with 99.99% of protection efficiency.

These results can be probably explained by the fact that owing to their homogenous dispersion into the polymer matrix, graphene nanosheets can play a critical role as an additional physical barrier which will increase the diffusion path of the ions from the corrosive media inside the hybrid coatings.

Fig. 1A: EIS diagram of uncovered E24 and E24 covered with GN@ppHMDSO coatings with different percentage of graphen(0.5 & 1 wt%). Fig. 1B: Magnification of the 1st part of Fig 1A.

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Abstract ID: 593

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Household and large-scale energy storage systems

Keywords: Energy Harvesting, Intercalation, ERG

Exfoliated and Reassembled Graphite Electrodes for Hygroelectricity

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Exfoliated and reassembled graphite (ERG) [1] is a new, high-aspect-ratio macroscopic material displaying useful chemical, interfacial, electrical, and thermal properties. Its application to make both electrodes in a hygroelectricity (HE) cell demonstrated the possibility to build large-scale, low-cost devices for distributed, autonomous energy production, including remote environments like humid forests. However, it is necessary to increase HE cells' output by some orders of magnitude to make them useful, which requires a model for their operation. We found a theoretical basis for HE cells in a usually neglected area of classical chemical thermodynamics, that is, electric potential gradients' effect on reaction Gibbs energies within a multiphase system [2]. The chemical effects of electric potential variations are widely explored in electrochemistry but not often in other areas. Most researchers assume the electroneutrality paradigm, notwithstanding the abundant evidence showing the existence of potential gradients in any interface. In the HE cell, the negative electrode owes its charge to adsorbed hydroxide ions while hydronium ions charge the positive electrode. The result is an electrostatic contribution to the reagents' Gibbs energy that increases with the potential difference between the electrodes. The outcome is the less-positive Gibbs energy for the water-splitting reaction that becomes spontaneous when the HE cell voltage reaches 1.63 V. The literature does not yet show HE cells producing such voltages. Still, current results in the >1 V range correspond to equilibrium constants higher than 10^-12, thus explaining the continuous delivery of electric current by the HE cells.

A new finding is the positive temperature coefficient of HE cells' power output, implying that the cell operation's reaction is endothermic. Among the candidate reactions that can take place in HE cells, the water-splitting reaction is endothermic, while metal or carbon oxidation reactions are exothermic.

The present results show that the HE cell could also become a source of hydrogen and oxygen released at the electrodes, but it is not as easy as collecting current from the electrodes.

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Abstract ID: 594

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster/Oral Presentation

Topics: Graphene, Mxenes and other two-dimensional materials for biomedical and healthcare applications

Keywords: Fusarium oxysporum, Entomo-pathogenic fungus, Silver Nanoparticles, Fungal Nanoparticles, Aedes mosquitoes

Fusarium oxysporum silver nanoparticles; their characterization and larvicidal activity against Aedes mosquitoes

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Fusarium oxysporum is an entomo-pathogenic fungus and it has anti-biological activity against mosquito larvae. Aedes mosquitoes are responsible for the spread of important diseases to human. Chemical application against mosquitoes is not eco-friendly and the flies are evolving to be resistant against the drugs. There is need to adopt biological control strategy against these mosquitoes. In the present study, we cultured a local isolate of Fusarium oxysporum from soil samples which was initially identified on the basis of morphology and then confirmed through PCR. A product of 339 bp was amplified from ITS gene of the fungus and then also got sequenced. In phylogenetic analysis, our sequence was in clad with Fusarium which was isolated from the body of a mosquito. Local Fusarium oxysporum was cultured and silver NPs were prepared. UV-Vis analysis depicted a broad peak at 420 nm wavelength and a narrow peak at 310 nm. X-Ray diffraction patterns of NPs indicated the existence of sharp diffraction peaks at 2 θ angles of 32.19°, 45.55° and 64.27° that can be indexed to the (101), (200) and (220) facets of silver which agree with the values reported for fcc lattice of silver NPs in JCPDS. The SEM micrograph showed well-defined spherical NPs; which were smooth, isotropic and poly-dispersed, ranging from 10 nm to 200 nm. The ZP measurements and poly-disparity index of 0.16 by DLS revealed a low variability of particle size and exhibited a good physiochemical stability of biosynthesized AgNPs. In FTIR spectrum of biosynthesized AgNPs, strong bands were analyzed at 3280 cm-1 and 1635 cm-1. Fusarium oxysporum NPs enhanced the anti-biological activity by killing Aedes larvae 7 hours earlier than F. oxysporum without NPs. Biological control through entomo-pathogenic fungi can be the best alternative to chemical method in order to control the mosquito population.

Abstract ID: 595

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Polymeric composites

Keywords: Polymer Composite Materials, Glass Reinforced Plastics, Thermosetting polymers, Modulus of Elasticity, Thermo-Relaxation

The effect of prolonged exposure to elevated temperatures on the deformability and relaxation of the structure of some thermosetting polymer binders

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Present work is devoted to studying the effect of relatively prolonged exposure to elevated temperatures on the change in the deformability of some thermosetting polymer binders and glass-reinforced plastics (GRP) used for the manufacture of composite structures, such as GRP shells of chimneys and gas flue ducts of industrial enterprises. Such structures during operation are exposed to the long-term combined action of mechanical loads and elevated temperatures. The following types of binders and composites were considered: epoxy resin with an anhydride curing agent, including modified with microsized mineral fillers and nanosized carbon tubes; phenolic resin of the resole type; epoxy-phenolic compositions; as well as some of unidirectionally GRP. All binders and composites were cured at elevated temperatures.

As a result, the effect of holding at temperatures from 160 to 240 °C on the elastic modulus of the specimens in bending, as well as on the nature of the weight loss, was investigated. In this case, the loss of mass did not occur because of thermo-oxidative destruction; the rate of weight loss decreased when held at a constant temperature, and the sample mass is stabilized. It was found that the change in the modulus of elasticity correlates with the loss of mass of the samples. It is assumed that this is due to temperature stabilization (relaxation) of the cured binder structure, which has a domain character. The stabilization (relaxation) of the structure is presumably physical rather than chemical in nature. The following research methods were used in work: static three-point bending, dynamic mechanical analysis, thermogravimetric analysis, spectral analysis, scanning electron microscopy.

The data obtained can be used to predict the thermomechanical SSS of structures at various stages of their life cycle, as well as for artificial regulation of SSS of structures (for example, creating prestressing) by means of their heat treatment under certain conditions. The study is aimed at developing a concept that describes the relationship between the laws of formation of the thermomechanical stress-strain state (SSS) of composites with mass and energy entropy.

Abstract ID: 596

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Dielectric materials

Keywords: Carbon fibers, composites, electromagnetic absorption, anechoic chamber, dielectric properties

Carbon fibers based epoxy foam composites: from dielectric characterization to electromagnetic absorption application

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Due to the rapid development of electronics and telecommunications, protection against electromagnetic waves has become an active area of research, and the intensification of protective materials usage is reflecting the market needs and the great demand of such products. The form and composition of electromagnetic absorbers are various and depend on the application under consideration. The typical absorbing materials used in the market have either flat or pyramidal forms. Pyramidal absorbers made of flexible polyurethane foam impregnated with a solution containing carbon particles are currently the most used materials for anechoic chambers. However, the carbon particles deposited inside the pores of the foam remain dangerous for human health due to their high volatility and nanometer sizes. This paper presents an alternative electromagnetic absorbing material developed from rigid epoxy foam and carbon fibers. The rigid foam was chosen because it can be machined with a complex geometry in order to enhance the absorption performances. Furthermore, our process enables the complete embedding of the fibers which prevents any leak. For this study, several composites of epoxy foam loaded with carbon fibers with length between 0.1 mm and 3 mm were achieved. Dielectric properties (permittivity and dielectric losses) of these materials were measured in 2 – 18 GHz frequency range. Therefore, numerical simulations of the reflection coefficient were performed to estimate the absorption performances of a pyramidal absorber and also a new designed geometry made of epoxy foam loaded with 0.5 %wt. of 3 mm carbon fibers. The simulation results showed remarkable performances: the reflection coefficient reached the mean value of – 45 dB. The measurement of prototypes in anechoic chamber confirmed the excellent performances with an equivalent even better reflection coefficient than the most used commercial absorber.

Key Words: Carbon fibers, composites, electromagnetic absorption, anechoic chamber, dielectric properties

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Abstract ID: 597

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Dielectric materials

Keywords: Glass foam, electromagnetic absorption, carbon, CRT, porous structures

Glass foam composites for high power microwave absorption

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Since early seventies, recycling chains of glass wastes were developed with a great success and glass containers are now widely recycled. But some types of glass, polluted with heavy metals, pose a tougher problem. Indeed, as hazardous materials, glass wastes from electronic industry (e-wastes) should be treated in specific recycling process. This is particularly the case of Cathode Ray Tubes (CRT) found in older style TV screens and monitors. Foam glass manufacture is a promising mode for re-using CRT glasses; depending on the foaming process, this cellular material combines low density, low thermal conductivity, excellent thermal stability and high rigidity. For this work, we focused our attention on EM absorptive properties of those glass foams based on cathode ray tube cullet. Inorganic additives can be used to reinforce the shielding properties in a specific spectral range. Indeed, when Carbon is used as the foaming agent, high dielectric losses are observed making of these foams a good candidate for EM absorbing applications [1,2]. In this work, we studied the impact of the glass cullet, the load rate and nature of the foaming agent on the density and the microwave behavior of glass foams. The thermal stability and the high power microwave absorbing application of these foams will be presented and discussed.

Key Words: Glass foam, electromagnetic absorption, carbon, CRT, porous structures

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Abstract ID: 598

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Dielectric materials

Keywords: Bio-sourced composite, electromagnetic absorption, carbon particle, anechoic chamber, reflection loss.

Bio-sourced composites for anechoic chamber absorbers

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Today, interest in microwave-absorbing material technology has been growing where continuous and increasing efforts have also been made in the last decade aiming at developing excellent electromagnetic wave absorbents. In anechoic chambers, the microwave absorbers usually used, are made from polymer matrix, such as polyurethane or polystyrene, which are produced by the petrochemical industry [1]. These materials are pollutants and their recycling is often very complicated.

In this work, we proposed an original material made from a bio-sourced matrix, acting as a support for the absorbent load (here carbon black). In addition to the rot-proof nature of this matrix and its thermal and acoustic insulation properties, the use of this material was motivated by two other properties: its low density and its fire resistance; two properties necessary for its use in anechoic chamber.

In this work, the dielectric characterization of the materials, with different compositions in carbon black, is presented and revealed very interesting dielectric properties with regard to the intended application: namely a low permittivity associated with high dielectric losses. The simulation of pyramidal absorbers, using measured properties, is done in order to choose the best composition for the achievement of a pyramidal prototype. The measurement of the absorber prototype showed excellent absorption performance for a normal and oblique (30°) incidences of the electromagnetic wave. Very low reflection (Γ <-40 dB) is obtained over a wide frequency range (between 3.5 GHz and 17 GHz). The prototype of Bio-sourced based absorbent also showed, for certain frequencies, better absorption performance than those of a commercial absorber with the same geometry.

Abstract ID: 599

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Dielectric materials

Keywords: Epoxy foam, Long carbon fibers, electromagnetic absorption, Low density, Multilayer absorber, dielectric properties.

Long carbon fibers loaded ultra-porous epoxy composite for planar microwave absorber materials

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Recently, absorber materials are being used widely in several applications, for example, electromagnetic compatibility, stealth and anechoic chamber etc... However, absorption in a wide frequency range, especially low frequencies, is still a constraint for such applications, and materials with significant thickness are often necessary to guarantee an acceptable absorption. So, today, the challenge for these absorbers is to obtain the best compromise between three factors: thickness, mass and performance.

In our team, a new absorber material made from rigid epoxy foam filled with a very low concentration of carbon fibers (CFs) is developed in order to replace the flexible polyurethane foam currently available as commercial absorber. This solution has been proposed in order to compensate the flexibility of these commercial absorbers which limits the precise machining process, and therefore the use of complex geometries to improve absorption performance. Our results show a very good microwave absorption performance of our materials compared with the commercial one. However, the density of the proposed material remains one of the restraints that must be optimized.

In this work, a promising methodology to fabricate ultra-porous CF/epoxy foam composite with a very high EM absorbing performance is presented [1]. The results show that the pore size and the density of the composite can be controlled; here, the material density can be reduced by half compared to the standard density of used epoxy foam. Furthermore, samples with different CFs loads, with different lengths, are elaborated and characterized in free space in order to investigate the influence of CF length and cell structure on dielectric properties of composites [1, 2]. The reflection coefficient and dielectric properties were extracted and compared with those of the dense CF/epoxy foam. Moreover, the suitable properties that ensure an impedance gradient are selected to make a multilayer prototype composed of 5 layers. The simulation and measurement of this very lightly loaded multi-layer prototype were compared over the wide frequency band 2-16 GHz; results were compared to those of the dense CF/epoxy foam multilayer and also to those of commercial multilayer absorber.

Abstract ID: 600

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Photonic devices and applications

Keywords: Strain, Integrated Photonics, Tensile strain, work function, 2D materials, TMDCs, photodetector, microring resonator

Strainoptronics: 2D materials with a twist

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Strainoptronics is an emerging concept that allows to manipulate and hence engineer a plurality of materials properties such as the bandgap, mobility, and Schottky barrier height for example. 2D materials are especially utilizable for strainoptronics given their low dimensionality leaning to a strong (2-4%) 'strainability'. In this presentation, I will share our latest explorations and device demonstrations including (a) an efficient TMDC photodetector at 1550nm wavelength on Silicon PICs [1, see right figure], (b) engineering the Schottky barrier height and reducing the bandgap by 200meV [2], and (c) showing scaling-length-theory based slot detectors with a potential for high gain-bandwidth-product photodetectors [3]. In detail, in integrated photonics, specific wavelengths are preferred such as 1550 nm due to low-loss transmission and the availability of optical gain in this spectral region. For chip-based photodetectors, layered two-dimensional (2D) materials bear scientific and technologically-relevant properties such as electrostatic tunability and strong light-matter interactions. However, no efficient photodetector in the telecommunication C-band has been realized with 2D transition metal dichalcogenide materials due to their large optical bandgap. Here, we demonstrate a MoTe2-based photodetector featuring strong photoresponse (responsivity = 0.5 A/W) operating at 1550 nm in silicon photonics enabled by strain engineering the 2D material. Unlike Graphene-based photodetectors relying on a gapless band structure, this photodetector shows a ~100X improved dark current, enabling an efficient noise-equivalent power of 90 pW/Hz0.5. Key Words: tensile strain, work function, 2D materials, MoTe2, photodetector, SOI.

Abstract ID: 601

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanomaterials and Nanotechnology

Keywords: PMMA/Fullerene C60 nanocomposites, Spectroscopy, Nanophotonics

Investigation of PMMA/C60 nanocomposites as nanophotonic materials for potential medical application

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Nanocomposites made of PMMA - Poly(methyl methacrylate) with different concentrations of fullerene C60 proved to have interesting optical properties and thus may serve as a good new material for spectacles. Because the structural properties of PMMA/C60 complex depend on the arrangement of methyl methacrylate (MMA) and C60 molecules, several nanocomposites (PMMA/C60) having different concentrations of fullerenes (0.025 wt.%, 0.05 wt.%, 0.075 wt.%, and 0.1 wt.%) were created and characterized by Magnetic Force Microscopy and UV-VIS spectroscopy. It is demonstrated that the structure of the complex directly correlates to the ratio of unpaired/paired electrons within the material. Also, Magnetic Force Microscopy was used to demonstrate the influence of different concentrations of fullerene molecules in PMMA on the attraction and the repulsion forces and consequently on the complex structural and optical properties. Based on investigation it is demonstrated that the PMMA/C60 complex with 0.025 wt.% concentration of C60 has the best structural and optical properties to be applied as a new material for spectacles. Based on UV-VIS Spectroscopic analysis in the domain of 380 to780 nm this concentration reduces UV and high blue energy light by more than 60%. Further, spectroscopic analysis of the influence of diffuse and linearly polarized light was done in domain 200-1100 nm, while the influence of green and red light before and after the interaction was separately done. It is demonstrated that the total difference of 42.26%, between diffuse and linearly polarized light of the same source of light, before and after the interaction with C60/PMMA complex exists. Analyzed experimental data performed by scanning tunnelling microscopy, strongly indicating that during C60-light interaction, exciton, as quantum 0D cavity phenomenon, is created that makes strong coupling with photons, creating polaritons. The hyperpolarizability property of C60 and photon half-quantization of its optical angular momentum create a new type of illumination (sunflower shape). Based on obtain results, the initial ophthalmological study, based on 50 volunteers, in the field of contrast sensitivity was conducted, and obtained positive results indicate that more, both scientific and clinical medical investigation of C60-light interaction, are needed.

Abstract ID: 602
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Carbon/Carbon Composites
Keywords: Laser Scanning, Flexible sensor, Carbon film sensor

Laser written flexible touch-pressure sensor array based on polyimide substrate

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Flexible electronic sensors processed through straightforward laser written nanomaterials have shown promising results with unique functionality. Compared to conventional electronics that are based on rigid substrates, flexibility of the polymer materials offers thin, lightweight, low-cost, mechanical stability, and conformability. The most widely used polymer substrates for flexible electronic devices include polyethylene terephthalate (PET), polyethylene naphthalate (PEN), and polyimide (PI). Among these, PI has been a strong candidate for interfacing with flexible printed circuit board electronics due to its high thermal stability, excellent mechanical stability, and dielectric properties. Thus, flexible electronics devices with PI as a substrate material have been widely reported. A very interesting point about the PI is its ability to convert intrinsic hydrocarbons into highly cross-linked carbon structures when interacted with laser. This process is enabled either by Photothermal or photophysical or even both. On the other hand, elemental carbon in different structural forms have been synthesized to fabricate various electronic devices and sensors due to their unique functional properties. Despite its unique features, straightforward synthesis, and most importantly patterning, of high quality (high conductivity) carbon structures in a scalable approach is quite challenging. To overcome this, lasers have evolved to directly write desired carbon patterns on polyimide substrates without any additional process or treatment to the substrate.

Herein, we report a flexible touch-pressure sensor with polyimide as a substrate and laser-treated carbon patterns as an interconnect and sensing elements. The laser-treated carbon film has a minimum sheet-resistance of 100 Ω/□ at a laser scanning speed of 100 mm/s, hatch spacing of 1 µm and repetition rate of 100 kHz. The sensor works based on the mutual capacitive coupling between two pair of electrodes that are of a loop and disc form. The approach also allows for the detection of proximity, touch and pressure, to enable a complete mapping of the sensor surface.

Abstract ID: 603

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: Carbon dots, hibiscus sabdariffa, polystyrene matrix, luminescence properties.

Green synthesis of luminescent Carbon Dots from Hibiscus Sabdariffa and its application in polymer matrix

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Carbon Dots (CDs) are new carbon-based nanomaterial, which is an abundant and generally nontoxic element, therefore they are attractive for hydrophilic applications. CDs, just like inorganic semiconductor nanoparticles (Quantum Dots) exhibit tunable fluorescence emission. Several techniques for CDs synthesis have been reported, such as pyrolysis [1], carbonization of polymer clusters [2], laser ablation, etc. There are numerous research about CDs synthesis from waste natural sources from fruit juice, fruit and a great variety of natural products [3] which are highly composed of carbon. Natural sources contain different organic functional groups that allows surface passivation during the CDs synthesis process and consequently, luminescent properties are showed with no functionalization treatment after said procedure.

In this work, CDs were obtained for first time, by easy and cheap calcination method, from hibiscus sabdariffa. This plant is species of Hibiscus genus, which is a liable for red to pink colors range as a result of existence of anthocyanin [4] and can be used to prepare herbal tea as medicinal treatment of different diseases, since its extracts are rich in anthocyanin compounds, ascorbic acid, flavonoids and hibiscus acids, which are water soluble.

CDs obtained were used in a polystyrene (PS) matrix, where mechanical properties are considerably improved, and luminescence properties are observed.

Abstract ID: 604
Symposium 4: Functional Composite Materials (FCM)
Poster/Oral Presentation
Topics: Nanocomposites
Keywords: CeO2, TiO2, Heterojunction, Photoelectrochemical performance

CeO2 nanoparticles on TiO2 nanorod: a Heterojunction with efficient Photoelectrochemical performance

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Photocatalysis is a process in which a photoactive material produces charges by absorbing light, which paves the way to harvest solar energy mediated by chemical reactions. TiO2 is among the most investigated photocatalysts because of its suitable band positions, chemical and thermal stability, biocompatibility and ease of availability[1]. However, its applications are restricted by the limited absorption in the UV region (which is only 5% of the full solar spectrum) owing to its wide band gap (anatase 3.2 eV and rutile 3.0 eV) and high recombination due to poor charge separation. On the other hand, CeO2 with a more negative conduction band position and lower band gap (~2.92 eV) is one of the most efficient companions of TiO2, leading to suitable band alignment and enhanced visible-light sensitivity in a CeO2-TiO2 heterojunction[2]. Here, we prepared the heterojunction by a two-step hydrothermal method. At first, TiO2 nanorods vertically grown on FTO coated glass substrate was synthesized by hydrothermal method, which especially helps to overcome grain boundary related issues and provide effective unidirectional charge transfer pathway. Then CeO2 was coated hydrothermally on TiO2. FESEM image of the CeO2 coated TiO2 nanorods is shown in Figure 1. An in-depth study of the optical, electronic and photoelectrochemical properties of this heterostructure were carried out to investigate the influence of heterojunction formation, preparation condition and processing variables on the system performance. The results of this work will be presented.

Fig. 1 FESEM image of CeO2-TiO2 nanostructure

Key Words: CeO2, TiO2, Heterojunction, Photoelectrochemical performance

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Abstract ID: 605

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: Monolithic TiO2 nanoparticle-based aerogels, Gas-phase nitrogen doping, Visible-light active photocatalysts, Photocatalytic H2 production

Gas-phase nitrogen doping of monolithic TiO2 nanoparticle-based aerogels for efficient visible-light-driven photocatalytic H2 production

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Hydrogen production using abundant solar energy and semiconductor photocatalysts holds significant potential as a clean and sustainable energy system. Macroscopically sized aerogel monoliths synthesized from preformed anatase nanoparticles are promising three-dimensional photocatalysts due to their immense surface area, high porosity, translucency, and the nanoscale characteristics of the semiconducting crystalline building blocks. Recent studies showed that such titania aerogels decorated with metals are effective for gas-phase photocatalytic CO2 reduction and H2 production [1, 2]. However, TiO2 nanoparticle-based aerogels remain limited to UV-driven photocatalysis due to the intrinsic wide bandgap (3.2 eV). To increase conversion efficiency from solar energy to H2 production, visible-light sensitization is necessary. Here, we present a facile method for the doping of the aerogel monoliths postsynthetically to make them visible-light active for H2 production. A CVD gas-phase reaction and plasma utilization at low temperature provided efficient nitrogen incorporation into preformed TiO2 aerogels without affecting their initial properties. The nitridation improves the optical absorption and charge separation efficiency through an appropriate balance between doping amount and coexistent defects. In comparison to the non-doped sample, the nitrogen-doped aerogels show a significant enhancement in visible-light-driven photocatalytic H2 production (3.1 mmol h-1 g-1) with excellent stability over 5 days. Our approach of gas-phase nitridation of preformed aerogel monoliths offers a powerful tool to improve their properties as visible-light active photocatalysts.

Abstract ID: 606

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Porous and cellular materials

Keywords: Graphene, Hexagonal Boron Nitride, Aerogels, Foams, Photonics, Actuators

Multi-Scale Materials by Effective Assembly of 1D and 2D Nanomaterials

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The fabrication of macroscopic and multi-scaled assemblies (such as sponges, foams, aerogels, etc.) from Graphene and related 1D and 2D nanomaterials is an extensively studied field due to their broad range of applications, such as in electronics, energy storage, catalysis as well as environmental protection. However, transferring the nanoscopic functionality of these unique materials into the macroscopic world is still challenging to achieve. In the here presented study, we demonstrate the versatile fabrication of multi-scaled framework architectures, composed of 1D and 2D nanomaterials, such as Graphene [1], hexagonal boron nitride (h-BN) [2], MXenes and carbon nanotubes [3]. With porosities in the order of 99.99% and densities as low as 0.2 mg/cm³ the properties of these so-called aeromaterials are determined by the nanoscopic functionality of the source material, enabling new applications. We demonstrate, that a multi-scaled material system composed of interconnected hollow h-BN microtubes, with a wall thickness well-below 25 nm, enables a novel class of high-brightness and efficient laser-based light sources. [2] The as-synthesized foam-like material forms a disordered and non-absorbing photonic network with thinly spread Rayleigh-type scattering centers, enabling a high degree in multiple light scattering. [4] Last but not least, we demonstrate that by exploiting the extreme low heat capacity of graphene-based aeromaterials cm3-sized gas volumes can be repeatedly and rapidly heated with heating rates beyond 300000 K/s and repetition rates of ~10 Hz. These "electrically powered explosions" demonstrate a reversible and environmentally friendly alternative to conventional chemical explosions, beneficial for applications in the areas of microfluidics, pneumatics, soft-robotics, propulsion systems, and thermoacoustics.

Abstract ID: 607
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Natural Fibre Composites
Keywords: cellulose, copper, electrically conductive paper, electroless synthesis

Towards electrically conductive wood: Synthesis of copper impregnated cellulose fibers and their processing into conductive paper

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The use of biodegradable and non-toxic cellulose as a renewable alternative to plastic in electronics is a promising way to decrease the environmental pollution. Unfortunately, cellulose lacks one of the key properties for such applications, namely electrical conductivity. Here, we report the complete impregnation of macroscopic cellulose fibers with copper nanoparticles using a simple, fast, gram scalable, electroless and catalyst-free liquid-phase approach. Addition of more precursor to the ongoing reaction makes it possible to tune the amount of copper nanoparticles inside the cellulose fibers, and thus to control the electrical conductivity of the final product. By simple vacuum filtration, the copper-impregnated fibers can be processed into self-supporting, paper-like membranes, whose electrical conductivity can be improved by slight pressing. The fiber-like morphology in these composites is fully preserved after pressing, leading to a high in-plane conductivity of 10’105 ± 751 S/m. By equipping cellulose with electrical conductivity, the functional properties of this renewable material are significantly extended, making it now attractive for a wide range of emerging applications in electronics and electrocatalysis.

Abstract ID: 609

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Photonic devices and applications

Keywords: Optofluidics, Nanophotonics, Biosensing, SERS

Partial Leidenfrost Evaporation-Assisted Ultrasensitive Surface-Enhanced Raman Spectroscopy in a Janus Water Droplet on Hierarchical Plasmonic Micro/Nanostructures

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The conventional methods of creating superhydrophobic surface-enhanced Raman spectroscopy (SERS) devices are by conformally coating a nanolayer of hydrophobic materials on micro/nanostructured plasmonic substrates. However, the hydrophobic coating may partially block hot spots and therefore compromise Raman signals of analytes. Here, we report partial Leidenfrost evaporation-assisted fast enrichment of low-concentration analytes in water droplets on hierarchical plasmonic micro/nanostructures, which are fabricated by implanting nanoantennas on carbon nanotubes-decorated Si micropillar arrays. In comparison with natural evaporation, partial Leidenfrost-assisted evaporation provides a levitating force to maintain the analyte droplet in the Cassie-Wenzel hybrid state. In this process, the continuous shrinking circumferential rim of the droplet, which is in the Cassie state, towards the pinned central region of the droplet, which is in the Wenzel state, results in a fast concentration of dilute analyte molecules on a significantly reduced footprint within several minutes. Partial Leidenfrost droplet can reduce the final deposition footprint by 3-4 orders of magnitude and enable ultrasensitive detection of nanomolar analytes because this type of hierarchical plasmonic surface has densely packed plasmonic hot spots with SERS enhancement factors (EFs) exceeding 107. Partial Leidenfrost evaporation-assisted SERS sensing on hierarchical plasmonic micro-/nanostructures provides a fast and ultrasensitive biochemical detection strategy without the need for additional surface modifications and chemical treatments.

Key Words: Optofluidics, Nanophotonics, Biosensing, SERS

Abstract ID: 610

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Bio-inspired design of composites

Keywords: Spider Silk, Soft Matter, NMR, cryo-TEM, Molecular Dynamics

Spider Silks as Model Systems for the Design of Functional Protein-based Materials and Composites

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Producing synthetic materials that exhibit the outstanding physical, mechanical and functional properties of spider silk is one of the Holy Grails of Materials Science. However, researchers still lack the knowledge to reproduce the hierarchical assembly process of spider silk proteins from the liquid spinning dope to high-performance fibers in the lab. The physical and biochemical transformation processes that take place to fabricate these protein-based materials remains a complicated problem with numerous unanswered questions. The characterization of these structural and dynamic evolutions typically lack the combined experimental data that can link the atomic, molecular and meso- length scale events responsible for protein assembly into fibers. The aim of this research is to harness recent advances in magnetic resonance, cryo-TEM and simulation to develop models for the transformation of soluble silk proteins to materials that out-perform man-made systems. Solution and solid-state NMR data is being combined with data from cryo-TEM imaging and tomography and molecular dynamics (MD) simulations to begin connecting the atomic, molecular and nanometer length scales for an improved understanding of hierarchical silk formation (1).

Spiders do not produce just one type of silk fiber but, up to six distinct fibers that are all exceptional materials that vary in their mechanical properties with some tougher than Kevlar while others exhibit extensibility and elasticity analogous to rubber. Our lab is developing an understanding of the silk protein structure-function relationship that make these silks unparalleled in performance yet, highly diverse. The majority of spider silk studies have focused on the dragline silk because of its strength and toughness and ease in which it can be collected. However, prey wrapping spider silk is actually tougher than the highly touted dragline silk because of a unique a-helical coiled b-sheet hybrid nanofiber structure (2) and exhibits a novel hydration-induced b-sheet fiber cross-linking property that we believe will provide inspiration for a new type of functional biomaterial (3).

Developing an improved fundamental understanding of the supramolecular physiochemical assembly process that enables the production of these natural materials and the global structure-function relationship across the various silks will impact applications in the defense, medical, industrial and space exploration sectors.

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Abstract ID: 611
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Smart Composites
Keywords: Stimuli-responsive materials, complex systems, soft robotics, smart materials

Pathway to "Intelligence": Using Stimuli-Responsive Materials for Constructing Self-powered Autonomous Functional Systems

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Intelligent systems are characterized by their ability to sense their environments, analyze surrounding signals, and provide a logical response. Intelligence is exhibited in many complex biological systems (e.g., human beings and animals) and electronic-based machines (i.e., artificial intelligence). On the other hand, materials (e.g., bricks) are generally regarded as static, passive, and far from being considered as "intelligent".

This presentation discusses the approach of using stimuli-responsive materials as basic building blocks for constructing self-powered autonomous "intelligent" systems. "Intelligent" systems usually consist of a combination of functions: the analytical processing functions, regulatory functions, and practical functions for responding to their surroundings. Stimuli-responsive materials are used to construct these types of stimuli-responsive functions via the combination of smart composites, physical-chemical phenomena, reaction, and design. For the stimuli-responsive analytical processing functions, we showed that the combination of a stimuli-responsive hydrogel and an asymmetric unsteady-state reaction-diffusion process allows the material to perform calculus: the temporal derivative of concentration of the medium. Hence, we showed that materials with simple designs can directly perform advanced mathematical functions. We further showed that assemblies of stimuli-responsive hydrogels with simple designs can perform the functions of multiple logic gates for integrated circuits. For stimuli-responsive regulatory functions, stimuli-responsive hydrogels are designed to perform the functions of gating and self-amplification. For stimuli-responsive practical functions, stimuli-responsive hydrogels are found to produce large amounts of force onto their surroundings. Despite being soft materials, these stimuli-responsive hydrogels are able to grip onto loads that are ~10,000 times more than their own weights. By functionalizing the surface of the stimuli-responsive hydrogels, they are shown to be able to target, capture, and rupture cancer cells. Self-powered autonomous "intelligent" systems can thus be created by combining the different types of specifically designed stimuli-responsive functions for carrying out complex analyses and operations for a wide range of applications.

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Abstract ID: 612

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Carbon, Quantum Dots, Emission, Photoluminescence, Optical devices, Energy Harvesting

Electrochemical synthesis of Carbon Quantum Dots and their Photoluminescence Trend

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Carbon Quantum Dots (CQDs) were synthesized through a sodium hydroxide-assisted electrochemical approach with no addition of any chemical treatment at the finish of the electrochemical procedure and using graphite pencils as carbon source. This route provides a convenient, facile and green method to prepare CQDs bye one step. The selected electric current densities used in the electrochemical procedure were 50, 100, 150 and 200 mA/cm2. The CQDs were characterized by images of Transmission Electron Microscopy (TEM), optical absorption and photoluminescence (PL) spectra. Analysis of TEM image of one carbon nanoparticle shows an average lattice spacing of 0.21 nm, this value matches well with the in-plane lattice spacing of graphene (100 facet). The absorption study showed non-monotonic behavior of absorbance intensity with the electric current density increasing. The PL emission peaks show redshift accompanied by a decrease in PL intensity when the excitation wavelength rise, with broadening ranging from 500 to 700 nm for all the electric current densities. This investigation contributes to obtain a better understanding of PL mechanisms in CQDs in order to offers considerable potential applications in several fields as bioimagen [1], ion detection [2], photoluminescence inks [3], coatings for light-emitting diodes [4]. photovoltaics structures [5], and co-sensitizers in dye-sensitized solar cells, [6]

Key Words: Carbon, Quantum Dots, Emission, Photoluminescence, Optical devices, Energy Harvesting

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Abstract ID: 613

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Ferroelectricity and piezoelectricity

Keywords: High Curie-temperature, Ferroelectrics, Piezoelectrics

Growth and properties of high Curie-temperature ferroelectrics

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Bi(Me)O3-PbTiO3 (Me=Sc3+, In3+, Yb3+) system has demonstrated the potential for generating piezoelectrics with high Curie temperature of above 450 oC, [1] high piezoelectric activity, and low temperature-property dependence, which will overcome the shortage of the relaxor-based single crystal piezoelectrics with a low Curie temperature (TC: 140 - 180 °C), such as Pb(Zn1/3Nb2/3)O3–PbTiO3 (PZNT) and Pb(Mg1/3Nb2/3)O3– PbTiO3 (PMNT) crystals, and meet the requirement for working under high temperature. In this presentation, we report the current research works and possible future development direction of Bi(Me)O3-PbTiO3 based advanced high Tc ferroelectric materials; especially, our report will focus on the development of Bi(Me)O3-PbTiO3 based crystals grown by the flux method and the thin films fabricated by chemical solution deposition. The structures, morphologies, performance of ferroelectrics and piezoelectrics of these materials are presented. Since the ferroelectric thin films have been intensively studied in recent years for their application in pyroelectric detectors, piezoelectric micro-sensors, and other micromechanical devices, this report especially presents the ferroelectric polarization and local domain switching behavior of the high-Tc Bi(Me)O3-PbTiO3 at the nano/micro-scale, measured by piezoresponse force microscopy (PFM) techniques.

Abstract ID: 614

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Functional Magnetic Materials

Keywords: Multiferroic Materials, Magnetic Properties, Phase Transition

Effect of Mn substitution on magnetic properties of Bi2Fe4O9 systems

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Multiferroics possess two or more orders, such as concurrent ferroelectric (FE) and anti-ferromagnetic (AFM) orders, which had considerably been attractive mainly due to their promising and potential applications in sensing, actuation, and digital memory. These materials also demonstrate various attractive physical phenomena that arise due to the strong coupling between magnetic and FE order parameters. The perovskite BiFeO3 (BFO) is such a material that has both FE (TCE=1103 K) and antiferromagnetic (AFM) (TN=640 K) orders. However, it is difficult to obtain pure-phase BFO; during the conventional synthesis process, the formation of a second phase of Bi2Fe4O9 had been reported to occur. Bi2Fe4O9 is a well-known multiferroic material that has been extensively studied over the past several decades. It exhibits an FE order at T=250 K and another AFM order (TN=260 K). [1] It is well known that the dopant could affect the magnetic and FE properties of this materials. To optimize or tailor the magnetic properties, in this work, we introduced the Mn substitution to research the effect of Mn dopant on the property of Bi2Fe4O9. The Mn-doped Bi2Fe4O9 powders had been successfully prepared by a soft chemical solution. XRD reveals that all doped samples are single phase, and their morphology have been analyzed by using SEM. The undoped Bi2Fe4O9 sample undergo an antiferromagtic transition at 250 K. With the Mn doping level increasing, the antiferromagnet transition temperature (TN) decreases. The magnetic moments of the samples decrease with higher Mn doping level.

Abstract ID: 615

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Solar Cells

Keywords: Nanosheets, Dye-sensitized Solar Cells, Hydrothermal Growth

TiO2 Ultrathin Nanosheets For Dye-Sensitized Solar Cells

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Dye-sensitized solar cells (DSSCs) have attracted intensive attention for their low cost and environmentally friendly comparing to the cells based on silicon1. Acting as photoanodes, the nanostructured Ti affects the overall performance of DSSCs and significantly improve the charge collection efficiency. The main purpose of this work is development of titania nanostructures and the corresponding composites by nanointerfacial engineering and chemical or physical routes for construction of flexible dye-sensitized solar cells (DSSCs), and investigation of the structure features and physics in the interfaces. In this work, ultrathin TiO2 nanosheets films were fabricated by hydrothermal growth of sodium titanate nanosheets, ion exchange of Na+ with H+ and topotactical transformation processes, and the structure, morphology, and photoelectronic properties were investigated. The prepared Nanocrystalline TiO2 films could be utilized as photoanodes for DSSCs.

Abstract ID: 616

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Sensors and MEMS: Materials and Devices

Keywords: SERS; machine learning; exosome; cancer diagnostics;

Surface Plasmonic Sensors for Biomedical Applications: aspects of light-biological matter interaction

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Surface plasmonics is an avenue of accumulating significant intensity of electromagnetic energy within a small volume of space immediately adjacent to a metal-dielectric (such as air) boundary. When matters such as biofluids are placed within the volume, various processes in the realm of light-matter interaction become possible. One such processes is surface enhanced Raman spectroscopy (SERS). In this report, aspects of the interaction between light and biological matters via Raman spectroscopy are examined from the perspective of diagnostic applications. In other words, what factors of such interaction contribute in which way to the diagnostic efficacy. The report is based on our journey in efforts to establish new diagnostic platforms for several disease types.

The journey began with the fabrication of plasmonic surfaces supplemented with graphene for facilitating quantitative SERS measurements [1]. The nano-engineered surface enabled single-molecule sensitivity and further the manipulation of single molecules via the mechanism of plasmonic tweezers [2]. One aspect of SERS scattering that potentially impact the specificity when studying biomolecules including protein, DNA and RNA comes from the relative orientation of the electric-field and atomic bonds [3]. The level of sensitivity combined with the level of specificity inherent to Raman scattering enabled the use of the plasmonic surface for biomedical diagnostic applications via SERS, a path our research group has followed during the past several years.

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Keywords: SERS; machine learning; exosome; cancer diagnostics;

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Abstract ID: 617

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Carbon, Quantum Dots, Emission, Optical devices, Photoluminescence

Temperature-Dependent Photoluminescence Spectra of Carbon Quantum Dots

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The mechanism for low-temperature photoluminescence (PL) emissions in Carbon Quantum Dots (CQDs) is investigated in detail, using PL spectroscopy as a function of temperature and excitation intensity. CQDs were synthesized through a sodium hydroxide-assisted electrochemical approach using graphite pencils as carbon source. Four different electric current densities were selected in the electrochemical procedure namely 50, 100, 150 and 200 mA/cm2. The CQDs were characterized by Transmission Electronic Microscope (TEM) with the aim to control the QDs shape and the average size. The optical absorption and photoluminescence (PL) spectra were investigated also in the four samples. Two bands were observed and are ascribed to the quantum confinement and surface states. Temperature-dependent photoluminescence measurements from 10 to 300 K were conducted. The two bands exhibit similar temperature dependence. The broadening of PL bands could be related to the strong electro-electron and weak electron-phonon interactions. The experimental results suggest that CQDs show similar temperature performance as metallic quantum dots but do not present the typical band gap shrinkage as in semiconductor quantum dots.

Key Words: Carbon, Quantum Dots, Emission, Optical devices, Photoluminescence.

Abstract ID: 618

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: 2D materials, defects, phase, synthesis, transition metal dichalcogenide

Defect Engineering in 2D Materials by Non-equilibrium Synthesis and Processing

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Defects in 2D materials significantly impact their structure and properties due to the ultrathin thickness and quantum confinement. In addition, defects in 2D materials can induce phase transitions, stabilize metastable phases, and give rise to the formation of new phases with different stoichiometries. Therefore, it is important to fundamentally understand the defect evolution and precisely control the type, density, and position of defects in 2D materials to tailor their properties and further introduce new functionalities. Here, I will demonstrate the nonequilibrium synthesis strategy to tailor the defect density and type in 2D transition metal dichalcogenides and the emerging properties for optoelectronic and electronic devices. Then I will introduce a defect-mediated phase transition by plasma irradiation in highly anisotropic 2D PdSe2. With in-situ scanning transmission electron microscopy characterization and theoretical calculations, the defect evolution and defect-mediated phase transformation in PdSe2 were studied at the atomic scale. Our results showed that depending on the concentration of Se vacancies in PdSe2, it could change to a variety of palladium selenides with different chalcogen contents. Through selective phase engineering, single material devices based on few-layer PdSe2 crystal with the new metallic phase as a seamless contact display significantly enhanced electrical performance due to the reduction in contact resistance and Schottky barrier height. Therefore, engineering defects in 2D materials is a promising way to tune their electronic properties and add new functionalities for future applications in optoelectronics and quantum information science.

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Abstract ID: 619
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Bio-composites
Keywords: Silk Fibroin; polymer sintering; biodegradable biopolymer

High-performance silk-based bioplastic from regenerated fibroin

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Due to the unique combination of properties such as mechanical strength and toughness, biocompatibility, biodegradability, thermal stability, and easy processability [1,2], regenerated silk fibroin has been used as a functional biomaterial, adopted when a positive interaction with living tissue is required. While a plethora of micro and nanoscale architectures of silk fibroin have been explored in literature - films, fibers, microparticles, and gels, building - larger, macroscale objects of fibroin has been challenging.

In this work we report a method to obtain a compact material form fibroin powder in a single compression mold step. We were able to optimize a fast, low temperature method to obtain large monoliths of solid – fibroin, reporting, for the first time a thermal – reflow at 40 °C for lyophilized silk fibroin [3]. With this technique large objects can be produced in few minutes with a high reproducibility. The mild forming conditions allow the possibility to incorporate temperature degradable bioactive additives. The possibility of post sintering molding through CNC machining or laser cutting allow the easy realization of user-defined shapes, making this biodegradable material suitable for several applications, included the design of biomedical implantable devices.

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Abstract ID: 620

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Embedded Nanoparticles and Nanocomposite Films

Keywords: Photonics, thin films, nonlinear optics

Nonlinear optical organic-inorganic nano-composite DAST/AAO

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The organic salt 4-N,N-dimethylamino-4'-N'-methly-stilbazolium tosylate, commonly known as DAST, has long been studied for its extraordinary nonlinear optical (NLO) properties [1]. In the bulk crystal form, it exhibits a high second-order nonlinear susceptibility $\chi^{(2)}$ that far outstrips that of many standard inorganic nonlinear crystals. This remarkable property of DAST has been widely exploited for THz generation, and recently further developed for second harmonic generation (SHG) in thin film forms, with results standing out in competition with even some of the best inorganic NLO crystals [2].

More recent experimental findings hint at the prospects of molecular engineering at the meso- or nano-scale for dramatically enhancing the nonlinearity via bond deformation.

Here we present a new series of further experimental investigations of the DAST molecular-engineering potential for enhancing its NLO properties through insertion of DAST into the nanopores of AAO thereby forming a novel organic-inorganic nano-composite. Underlying the heterogeneous incorporation is the creation of an intriguing interplay between a cylindrical stress built-in by Laplace's force that is inversely proportional to the diameter, the anisotropic ionic DAST, and an optical density of states and mode volume modified from that of bulk DAST by the local nanostructure.

The host AAO matrix is the anodized aluminum oxide (AAO) with nanometer-sized cylindrical pores perforating through the membrane. The DAST-AAO nano-composite films are subjected to 1064 nm nanosecond laser pulses and the SHG signal is measured as a means of assessing the molecular and nano-engineering effects on the NLO properties of the DAST. The SHG measurement was conducted in the reflection mode, necessitated by the sample inhomogeneity. Clear and substantial enhancements of SHG were observed in correlation with thermal annealing, attributable to recrystallization and bond deformation induced by the built-in stress and corroborated by additional tests under externally applied stress (by bending the films under test).

Acknowledgement: We are thankful to the support of AFOSR FA9550-19-1-0355 and ARO W911NF1420075; and to the DAST molecules synthesized and provided by Prof. X.D. Xu's group.

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Abstract ID: 621
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Carbon/Carbon Composites
Keywords: Nanocarbon, Phonon, Composite film, Thermal conductivity, Thermal rectification

Small-Nanostructure-Size-Limited Phonon Transport within composite films made of single-wall carbon nanotubes and reduced graphene oxide sheets

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Nanocarbon materials have been widely used for nanoelectronics and other energy-related applications.In the kinetic relationship, the phonon (lattice) thermal conductivity is given as $k_L \sim C_p v_g \Lambda$, with C_p as the phonon specific heat, v_g as phonon group velocity, Λ as phonon mean free paths (MFPs). Within general composite films made of reduced graphene oxides (rGOs) and carbon nanotubes (CNTs), the existence of many nanocontacts results in a k reduction but the loss in k can be overshadowed by the significant advantages of using bulk composites for large-scale applications. Detailed thermal analysis of composite films made of rGO and CNTs is still lacking, particularly for the individual in-plane thermal conductivity ($k_\parallel$) contributed from each constituent material within the complicated 3D nanocarbons. In this work, composite films consisting of rGO nanosheets and varied weight percentage of single-wall CNTs (SWCNTs) are synthesized and studied for their in-plane thermal conductivities, in which increased SWCNTs percentage leads to a reduced $k_\parallel$. Different from pristine graphene and other composite nanocarbon films with decreased thermal conductivities above 300 K, the in-plane thermal conductivities of our composite films are found to follow the trend of the specific heat of graphene from 100 K to 400 K, i.e., monotonously increasing at elevated temperatures. For investigated samples, the extracted $k_\parallel$ can be matched by a scaled curve for the product $C_p v_g$ summed up for all phonon modes that are computed for pristine graphene. This indicates that the rGO nanosheets contribute significantly to the $k_\parallel$ but their MFPs are largely restricted by the dense SWCNT-graphene junctions and additional graphene-graphene nanocontacts. Such a trend has seldom been observed for nanocarbon. This unique temperature dependence of thermal conductivities is attributed to the so-called small-nanostructure-size (SNS) limit, at which the phonon MFPs are simply restricted as the structure size. This SNS limit is often found at cryogenic temperatures where the majority bulk phonon MFPs are much longer than the sample size. The typical size of graphene sheets divided by SWCNTs is 70–120 nm for Sample #2, and 15–30 nm for Sample #6. These sizes are smaller than the majority phonon MFPs (>100 nm) in graphene so that the phonon transport within graphene sheets approaches the SNS limit. This results in $k \approx k_L$ following the SNS limit even up to 400 K. The highest in-plane thermal conductivity among samples with different synthesis conditions is 62.8 W/m·K at 300 K, which is significantly higher than amorphous materials with a similar temperature dependence of thermal conductivities. Such a high thermal conductivity, combined with its unique temperature dependency, can be ideal for applications such as flexible film-like thermal diodes based on the junction between two materials with a large contrast for their temperature dependence of the thermal conductivity.

Abstract ID: 622

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Dielectric materials

Keywords: microwave sintering; piezoelectric ceramic; impedance; Debye type relaxation

Effect of sintering temperature on impedance and electrical modulus of microwave sintered PZT for LTCC applications

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Piezoelectric ceramics are electro-mechanical transducers that get polarized when strained. The converse effect electrostriction is also true for these ceramics where in change in the dimensions of the ceramic is resulted when electric filed is applied. Lead zirconate titanate is one such piezoelectric ceramic. Ever since its' discovery in 1952 PZT has become invincible in sophisticated instruments due to its greater piezoelectric sensitivity, mechanical strength, chemical stability and easily tunable piezo-properties. An alternate to PZT in electronic industry is yet to be realized [1]. Though PZT is extensively studied reports on microwave sintered PZT are little to nil. In the present work, an attempt is made to study the dominant conduction mechanisms of microwave sintered PbZr0.52Ti0.48O3 (PZT) ceramic samples at different temperatures (800, 820, 840, 860, 880, 900, 920) are presented. Impedance and electrical modules studies are studied on the samples in the frequency range 100 Hz to 1MHz at different temperatures. Approximate analysis revealed Debye type relaxation behaviour at low frequency in all samples. Grain and grain boundary effects are observed in frequency dependent complex impedance plots (Z' Vs Z") and modulus plots (M' Vs M"). Anomalous behaviour is noticed for the PZT microwave sintered at 900oC which is attributed to the complete formation/densification of PZT at this temperature. Discussion on the dielectric properties of the ceramic samples estimated at optical frequencies is presented.

Abstract ID: 623

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Liquid electrolytes, ionic liquids, polymer electrolytes

Keywords: Key Words: Ionic Liquids, Melting Transition, Nanocarbons, Energy Storage

Phase transitions of EMIN TFSI ionic liquide (1-Ethyl-3-methylimidazolium bis (trifluoromethylsulfonyl) imide confined in nanocarbons

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Currently, a much research in electrochemistry is concerned with the effect of direct application of the ionic liquids as electrolytes for supercapacitors (SC) – the energy storage devices operating through the formation of an electrical double-layer, by simple separation of ions at the electrode/electrolyte interface. The high applicability of these systems results from their exceptionally fast charging/discharging time measured in few seconds. Due to the fact the operation conditions for SC require low temperatures, an important issue is an investigation of melting behavior of ionic liquid applied as an electrolyte.

We report the experimental studies of the melting behavior of 1 - Ethyl -3 - methylimidazolium bis(trifluoromethylsulfonyl)imide (EMIM TFSI); for this purpose the methods of dielectric spectroscopy (DS) and differential scanning calorimetry (DSC) in wide temperature ranges were applied. To investigate the structural properties of the system the temperature-controlled WAXS and Neutron Diffraction methods were adopted. The measurements of the complex permittivity of the studied EMIM TFSI allowed us to determine the relaxation of the system in wide temperature range from 140 K to 300 K. The results obtained from DSC and DS indicate that the ionic liquid on the heating process undergoes two phase transitions: solid-solid transition at temperature 230 K and the melting transition at 257 K, wherein the melting process is not homogeneous. Based on the structural studies results, performed in the temperatures range 10 K – RT, it was shown that in the temperature range 10 K-230 K EMIM TFSI forms a crystal monoclinic structure where the rotation motions of molecular groups are observed. At the higher temperature up to the melting temperature the crystal structure is undefined and the rotational motions of molecular groups are changed. The similar studies performed for EMIN TFSI confined in carbon micropores show that the melting process of IL in pores is unhomogeneous and melting temperature of IL decrease relatively to EMIN TFSI bulk melting point.[3]

Key Words: Ionic Liquids, Melting Transition, Nanocarbons, Energy Storage

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Abstract ID: 624

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Thin-film transistor, Piezoelectric device, flexible electronics, high-speed electronics, ultrasound detection.

Molybdenum disulfide (MoS2) based Thin Film Transistor for Ultrahigh Speed Detection of Ultrasound Waves

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Molybdenum disulfide (MoS2), as a semiconductor material, is of greater concern for delivering high-performance electronic devices for potential applications in detectors, transducers, energy conversion, optoelectronics, and sensors due to its high mobility, low noise level, and high robustness properties. Here, the MoS2 semiconductor is utilized as supporting electronics in form of a thin-film transistor (TFT) on a flexible platform to obtain high-speed detection of ultrasound waves. The proposed MoS2 based TFT is combined with the self-assembled piezoelectric device based on polyvinylidene fluoride trifluoro-ethylene P(VDF-TrFE) for ultrasound detection at high speed. The proposed flexible MoS2 based TFT shows high mobility of 17.5 cm2/Vs, and an on/off current ratio of ~105 with stable mechanical robustness properties under complex environments. Additionally, the switching properties of the proposed flexible MoS2 based TFT are measured at different frequencies (10 kHz, 100 kHz, and 500 kHz), revealing highly stable switching of the proposed device, thus, introduced as supporting electronics for high-speed detection of ultrasound waves. Next, the ultrasound waves are successfully detected in terms of transfer curve by connecting the self-assembled piezoelectric device with the proposed flexible MoS2 based TFT. The results show a linear behavior of ultrasound waves detection under different ultrasound waves along with a clear detection of ultrasound at different frequencies, thus, enabling a new platform for establishing high-speed measurements in the field of electronic devices and biomedical imaging tools.

Abstract ID: 625

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Photonic devices and applications

Keywords: Photonic quantum ring (PQR), angle-resolved light cone (ARLC), WGM

Noninvasive analyses for brain disease by monitoring angle-coherent spectra from photonic quantum ring laser of whispering gallery modes

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Noninvasive diagnoses by angle-resolved coherent tomographic infrared spectroscopy (ACTIRS) are presented, where 3-dimensional (3D) angle-resolved light cones (ARLCs) from photonic quantum ring (PQR) laser of whispering gallery mode (WGM) are employed. It is important that we analyze the return spectra optically, not photocurrent-converted as for conventional FNIRS, after the cortical, vascular or muscular diffuse brain paths, The unique angle-coherent multi-spectra will eventually lead to ionic or protein analysis associated with cranial tissue or arterial line before that is obtained only from uncomfortable brain MRI, CT or biopsy.

PQR laser location (L) and the track of an angle(e.g.,~30°)-resolved light cone (ARLC) where (C)-fiber probe can be placed at a selected point for detecting return signals of specific blue-shifted wavelength. Then about 3 cm penetration depths (BIOPAC's FNIRS sys. estimates) let us imagine an equilateral triangle of L – C (fiber probe) – T (target region), being a cross-section of a schematic ARLC (Fig.1a), agrees and roughly follows the blue-shifted diffuse paths (~30° inclination); PQR's spectral paths through frontal lobe (red and) blue diffuse paths are consistent with blue-shifted incident laser as shown in Fig. 1b. The paths consisting of heterogeneous media in general will need further investigations.

The PQR laser, a cylindrical mesa structure of active Ga(Al)As or InGaAs multi-quantum well (MQW) plane between top and bottom DBRs, functions as concentric quantum-wire emitters within the PQR's peripheral Rayleigh band of 2-dimensional (2D) MQW circles, which is associated by nature with traditional 2D WGM phenomena in x-y plane as explained by Lord Rayleigh in 1912. The PQR Rayleigh band plane is optically surrounded by new 3D whispering cave mode (WCM) regions due to DBRs. The systematic variations of intermodal spacing agree with a well-defined angular quantization rule, while the VCSEL peak, λ0, shows no spectral profile (Fig. 1b).

Figure 1: (a) (b)

Abstract ID: 626

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Sensors and MEMS: Materials and Devices

Keywords: Temperature Sensor, stretchable-gradient interconnection, biomedical device

Stretchable-Gradient Temperature Sensor System using Laser-induced Process

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Wearable epidermal sensor systems have gained more interest in healthcare monitoring devices with different sensor geometry and device architectures. Although the reported wearable sensors exhibit high-performance biological sensing but require a reliable sensor system design that can accommodate both sensor (soft) and circuit (hard) parts for accurately monitoring the facile information of biological signals. In this work, we report a novel structure of the temperature sensor inspired by nature (Kirigami-serpentine design that is 3D deformable and 2D stretchable) with stretchable-gradient interconnection electrodes for a wearable biomedical device to obtain long-term real-time body temperature. The proposed stretchable-gradient temperature sensor system is designed on a solution-based polyimide (PI) substrate where platinum (Pt) metal is utilized as a sensing material. The patterning of the proposed temperature sensor system has been performed by laser processing technique simply. The electrical and mechanical measurements with multiple testing processes are performed and the results show a linear response under different temperature scales and high robustness properties over various strain tests. A multi-layer wearable patch and a custom-built mobile application are designed to establish a conformable bonding to human skin and obtain wireless real-time monitoring of body temperature, thus, establishing a new approach towards real-time monitoring systems with high accuracy and stability over complex environments in the field of wearable electronics.

Abstract ID: 627

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Solar Cells

Keywords: Low-cost, low environmental impact, organic solar cells, sustainable manufacturing

Is push-coating the adequate solution to solve the sustainability issue of organic solar cells fabrication?

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Unlike silicon or GaAs based photovoltaics, organic solar cells can be printed at low temperatures and can be manufactured as semi-transparent or flexible devices. Therefore, they receive enormous attention as clean energy source for low-income countries or for energy sustainable cities. However, conventional fabrication of organic semiconductor thin films by spin-coating results in large amounts of hazardous solvent and material being released in the environment (Fig. 1). The work we present here focuses on a thin film fabrication process that considerably reduces the wastes generated during organic solar cell fabrication, which we call push-coating (Fig. 1) [1]. When a silicon elastomer is placed on top of a very small volume of semiconductor solution deposited on a substrate, the solution spreads between the elastomer and the substrate through capillary forces. The solvent then diffuses into the silicon elastomer which results in the formation of uniform semiconductor thin films.

Fig. 1 (included in the attached abstract): Schematic representations of the spin-coating and push-coating processes.

Using push-coating, the amounts of hazardous solvents and material employed can be reduced by 20 and 40, respectively, compared to spin-coating. Additionally, the hazardous solvent can be trapped into the elastomer and easily recycled. We verified that push-coated organic solar cells can yield similar performances to spin-coated ones when using conjugated polymer electron donors and fullerene acceptors [1,2]. However, the results obtained with non-fullerene acceptors are less straightforward and strongly depend on the crystallization dynamics of the semiconductors in the thin films. Nevertheless, our results clearly indicate that push-coating has a great potential for the fabrication of low-cost, green & sustainable organic solar cells.

Key Words: Low-cost, low environmental impact, organic solar cells, sustainable fabrication

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Abstract ID: 628
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Bio-composites
Keywords: nanocellulose, peptides, hybrid materials, gels

Nanocellulose-peptides gels: a hybrid platform for biophysical applications

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Nanocellulose (NC) shows several fascinating properties that render it a material of interest for a broad range of uses (1). NC hydrogels are easily produced by crosslinking the NC phase with either ions or molecules bringing a positive complementary electrical charge. The gelation mechanism permits to create biocompatible, optically transparent NC gels with tunable mechanical properties that, together with its chemical inertness and good biocompatibility, render NC as a candidate material for a number biophysical and chemical applications. NC gels have been proven effective as cell scaffolds, drug delivery and diagnostic devices (2,3). Here we show our latest results on the development of composites materials where the combined use of NC and peptides permits to tune the mechanical and water retention properties of the hybrid gels and enables the introduction of complementary chemical functionalization thanks to the use of ad-hoc designed peptides. Rheological, optical and structural analysis were conducted to unveil the relationship between materials structure and properties. Proof of concepts application of these materials in biochemical analysis and cell cultures are shown.

Abstract ID: 629

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: Bubble-free, electrolysis, hydrogen, effcient

Micro and Nano Structures that Enable 'Bubble-Free' Water Electrolysis that is Highly Energy Efficient

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Highly efficient electrochemical splitting of water into hydrogen and oxygen constitutes the most critical capability needed for the development of a future hydrogen economy based on renewable energy.1 In this work we demonstrate that direct conversion of water into hydrogen and oxygen gas, without the intermediacy of gas bubble formation, may notably decrease the energy required. We report the operation and performance of "bubble-free" alkaline electrolyzers with electrodes that combine catalyst layers containing high-performing water-splitting catalysts, with gas removal structures. The gas removal structures vigorously extract the gases as they are produced by the catalyst layer, before bubbles can be formed. In so doing, the energy penalties arising from bubble formation are avoided. At 80 oC, the best electrolyzer produced ~800 mA/cm2 at 95% energy efficiency (1.54 V) and ~400 mA/cm2 at 100% energy efficiency (1.47 V), relative to the Higher Heating Value (HHV) of hydrogen. These results constitute an ~20% increase in energy efficiency over present-day commercial alkaline electrolyzers.

Abstract ID: 630
Symposium 4: Functional Composite Materials (FCM)
Poster/Oral Presentation
Topics: Bio-composites
Keywords: Chitosan, β-Cyclodextrin, Cerium oxide, Environmental remediation

Synthesis of innovative chitosan-based functional composite adsorbents: Materials characterization and application in environmental remediation

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Restoration of the aquatic environment is nowadays a challenging task due to the presence of numerous contaminants commonly found in industrial effluents, lakes, and underground waters. Although several treatment methods have already been applied for water purification (i.e. adsorption processes), the utilization of functional composite materials as adsorbing agents is of great interest, mainly because of their structural properties that grant them exceptional adsorption abilities coupled with high mechanical strength. Notably, polysaccharides are a category of materials that have presented encouraging results in the adsorption of contaminants, with chitin along with its derivative, chitosan, being the most prominent ones. Chitosan, a biopolymer derivative of chitin, is a promising constituent for the synthesis of functional composites due to the presence of amino and hydroxyl functional groups in its structure. Materials consisting of chitosan are widely studied towards various applications including environmental restoration. Specifically, chitosan has been proven an effective adsorbent with high adsorption efficiency towards a variety of contaminants, such as heavy metals and organic contaminants. Consequently, great interest has been presented in the research for the synthesis of chitosan and chitosan-based functional composites and their application in the field of water purification via adsorption. The present study investigates the synthesis of several innovative chitosan-based adsorbents and aims to provide a comprehensive analysis of their structure and properties along with a detailed evaluation of their adsorption efficiency towards targeted water contaminants. Thus, chitosan coupled with cerium oxide or β-cyclodextrin functional composites will be produced by means of crosslinking, meticulously characterized by means of XRD, SEM, and FTIR analyses in order to assess their morphological structure and properties. Finally, the adsorption efficiency of the synthesized functional composites will be evaluated in the removal of specific contaminants, namely hexavalent chromium, indigo carmine, and brilliant black, from aqueous solutions by means of adsorption.

Abstract ID: 631
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Smart Composites
Keywords: shape memory alloys, analytical model, experimental tests, smart composites

Design and Characterization of Elastomer-SMA Composite Actuators

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Actuators based on Shape memory alloys (SMAs) are typically characterized by a high force/stroke ratio and can be activated by an increase in temperature, which is usually induced either by passing an electric current or applying direct heating [1]. SMA composite actuators are often designed as two-component systems with an agonistic-antagonistic relationship, where the main role of the second component is to act as a counter-balance and revert the actuator back to its original shape once it has been deactivated. Creating a composite actuator with reversibility properties involving SMA wires embedded in a soft matrix entails a delicate balancing act in which the appropriate material properties and volume fractions of the two components must be chosen carefully. The proposed design methodology ensures that the stiffness of both individual components is optimized to provide maximal actuation stroke and reversibility of the composite system. A simple analytical model, based on the geometric parameters and material properties of the single components, is proposed by the authors and may be used to design such composite actuators and to predict the actuation output and reversibility of these systems. The method was already validated against the literature models of SMA materials [2] providing satisfactory results [3]. In addition, we have also devised a fabrication method through which an elastomer-SMA composite based on this model may be produced and thus a fully-functional prototype actuator may be manufactured. By comparing the analytical predictions with the experimental results the precision and the applicability of the proposed method is assessed and discussed.

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Abstract ID: 632
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Processing and manufacturing technologies
Keywords: Laser ablation, sensors, flexible and stretchable electronics

Rapid laser ablation technique towards low-cost flexible and stretchable electronic devices for human-machine interactions

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Recently, flexible and stretchable electronic devices have gained huge attention to assist human-life in health care monitoring, assistive technology, and human-machine interactions. Moreover, these electronics could be conformally and comfortably attached to human bodies without producing any adverse effect on skins and while simultaneously maintaining sensing functionalities under significant deformations. Till now, the sensors fabricated by state-of-the-art conventional microfabrication techniques are highly expensive, time-consuming, mask dependent, incompatible with roll-to-roll processing, and involves hazardous chemicals. In contrast, sensors fabricated from one-step laser ablation technique are rapid, inexpensive, scalable, mask independent, user-friendly, and roll-to-roll compatibility greatly enhance the realization of low-cost electronic systems.1

Laser's technology has continued to grow its exceptional breakthrough contributions to the technology and is becoming ultrafast, user-friendly, and inexpensive every year. The programmable lasers ranging from nanosecond (1ns = 10-9 s) to femtosecond (1 as = 10-15 s) have been extensively applied to modify the surface/bulk of the materials like ablation, nano-welding, carbonization, scribing, drilling, and bulk heating for various flexible and stretchable electronic applications. Unlike ultrafast pulse lasers which interact surface in a timescale faster than lattice disorder, nanosecond lasers ablate materials by a thermal process. This thermal ablation causes a large heat-affected zone that may induce melt redeposition and shockwaves, leaving behind thermally induced defects such as cracks and chipping. Laser ablation termed as material removal by high-intensity laser pulses used to cut and scribe materials has been widely adopted to manipulate the surface appearance of materials for various needs.

Herein, we demonstrate the use of the pulsed laser ablation technique to fabricate various flexible and stretchable sensors, which include temperature, humidity, pressure, and electrophysiological. By systematically tailoring the physical properties of the active and substrate materials, various electronic devices with tunable mechanical and electronic properties can be achieved. This approach renders constructive insights for producing rapid, low-cost, mask-less, and scalable flexible and stretchable electronic devices.

Abstract ID: 633

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Natural Fibre Composites

Keywords: Fenugreek, Galactomannan, Liposomal Hydrogel, Self-emulsifying nano-delivery, Vitamin C, Pharmacokinetics

Fenugreek galactomannan as a novel biopolymer for the Self-emulsified Nanodelivery of Water-Soluble Nutrients with Enhanced Bioavailability

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Natural and food-grade oral delivery technologies suitable for wide range of pharma (capsules, tablets etc) and food (gummies, sachet, etc.) delivery formats capable of delivering nutrients with enhanced bioavailability are limited, unlike the lipophilic molecules. Fenugreek (Trigonella foenum greacum) is a popular kitchen spice and medicinal herb widely approved globally for food and nutritional applications. It is a rich source of highly sterically hinders galactomannans with a unique ratio of 1:1 galactose to mannose. It has already been used in the delivery of lipophilic molecules like curcumin. The present study was aimed at the development of novel hybrid hydrogel systems based on fenugreek galactomannans (FG) for the oral delivery of water-soluble nutrients like vitamin C with enhanced bioavailability. The unique physico-chemical characteristics such as rheological properties, swelling, mucoadhesive nature, amphiphilic property and stability of fiber and its hydrogel were evaluated and an ultrasound-mediated gel-phase dispersion technique was developed for the encapsulation of ascorbic acid liposomes into the galactomannan hydrogel matrix. The interaction between the liposomes and hydrogels were established by FTIR studies and the rheological, structural and morphological properties were also followed. It was found that the hydrogel can be dehydrated to fine free flowing powder suitable for storage and formulations and can be further rehydrated to hydrogel. The reversible hydrogels thus obtained was found to exhibit a cumulative release of ~88 % at 8 h, indicating the sustained-release of ascorbic acid at average particle size of 130±20 nm. The self-emulsified particles of vitamin C thus released from hydrogel matrix was found to offer better bioavailability and pharmacokinetics as evident from the prolonged residence time in the circulation and increased the concentration in plasma when supplemented to human volunteers at 500 mg/tablet. Thus, fenugreek galactomannan-based hybrid hydrogels were found to be an efficient green approach for the oral delivery of Vitamin C, which is an essential for the maintenance of body homeostasis, since our body cannot synthesize or store and hence require continuous supplementation

Abstract ID: 634
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Nanocomposites
Keywords: Nanocomposites core/shell, nanorods, surface functionalization.

Synthesis and Characterizations of 1D CdS/ZnS core/shell nanocomposites

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The growth of wide bandgap semiconductors like ZnS on the surface of narrower bandgap semiconductor CdS forming nanocomposites leads to the appreciable passivation that results in enhancement of the properties of the material. Because of the improved properties, core/shell nanoparticles are widely used in different applications such as biomedical, catalysis, electronics, photonics etc [1-4]. Herein, CdS/ZnS core/shell nanorods were successfully synthesised via three-step synthesis method-(a) solvothermal synthesis of CdS nanorods, (b) surface functionalization of CdS nanorods by using citric acid and (c) growth of subsequent ZnS shell. Different reaction time and molarity of Zn2+ precursor were tested to optimise the synthesis conditions. The as- prepared CdS/ZnS nanorods were used to study the structural and optical properties by XRD, UV-Vis spectroscopy, FT-IR and PL spectroscopy measurements. The XRD confirms the crystal structure of CdS/ZnS nanorods having peaks corresponds to the hexagonal and cubic structures of CdS and ZnS nanostructures respectively. UV-Vis absorption spectra having broad peak at ~505nm corresponds to the CdS in visible region and a small hump of ZnS at ~349 nm confirms the formation of ZnS shell over the core CdS and shows no significant effect of varying reaction time and molarity of Zn2+ on absorption peaks position. The PL spectra of CdS/ZnS core/shell nanorods exhibiting emission peaks centered at ~530nm, 485nm, 422nm and 407nm. The peaks at 530nm and 485nm are assigned to the sulfur vacancies in CdS and due to band edge emission in CdS whereas the peaks at 422nm and 407nm may be due to the CdS/ZnS interface or S interstitials and transition from surface sulfur vacancy to surface Zn vacancy respectively. Further, FT-IR spectra confirms the presence of Cd-S bond and Zn-S bond and shifting in bonds appears with increase in reaction time. Our present study provides a simple and cost effective technique to design the core/shell nanocomposites with application in optoelectronic devices.

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Abstract ID: 635
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Nanocomposites
Keywords: CdS:SiO2 nanocomposite thin films, room temperature LPG sensor, CdS nanodroplets, silica micro balls, pulsed laser deposition.

CdS Nanostructures for efficient room temperature LPG sensing

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The increase in casualties of liquefied petroleum gas (LPG: one of the highly inflammable gases) day by day all over the world due to its widely spread usage as a fuel gas in homes, workplaces, and industries including those of automobiles is becoming a serious concern and demands efficient room temperature sensor. This talk will comprises the review of room temperature (RT) LPG sensors using CdS nanostructure followed by the discussion on our experimental results on CdS:SiO2 nanocomposite thin films (CdS:SiO2 NCTFs)1. Our experimental results demonstrated that CdS:SiO2 NCTFs showed an efficient room-temperature sensor for LPG. Though, many successful efforts have been made to achieve a low operating temperature using a variety of nanomaterials and their hybrid structures/composite materials have even been demonstrated to work at room temperature (RT). 2-4 However, this particular feature is typically observed in CdS nanocomposites or CdS heterostructures. Pulsed laser deposited CdS:SiO2 NCTFs followed by thermal annealing display the morphology of CdS nanodroplets over micron-sized spherical balls of SiO2. The sensors of as-grown and annealed CdS:SiO2 NCTFs along with bare CdS thin films were prepared over Pt interdigitated electrodes. The sensing response of fabricated sensors in the presence of reducing gases, viz., LPG, H2, H2S, NO2 and CO2 was recorded by measuring the resistance of the films in air and gaseous environments. The highest response (~ 71% for 1000 ppm at RT) of present sensor was achieved for LPG with the response time and recovery time of 91 s and 140 s, respectively. The promising usage of present sensor for low-temperature regions as well was suggested by the sustainable response of the sensor up to 75℃ and then decreased. Besides, even after storage of 8 weeks, the sensor retained ~ 96% of its initial response, which strongly endorsed the ambient environment free sustainable performance of device. In spite of a low detection limit of 20 ppm at RT for LPG, sensor showed a significant response only at 50 ppm. Even though the simple fabrication technique RT operational fabrication of sensor with high sensitivity, low detection limit, low response and recovery times, and good reproducibility, the present LPG sensor is highly promising.

Abstract ID: 636

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Liquid electrolytes, ionic liquids, polymer electrolytes

Keywords: Ionic liquids, Europium, Heat Energy Conversion

Ionic Liquids for New Thermoelectrochemical Cells

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Due to technological progress and population growth, a huge increase in demand for energy is expected in the next years. However, energy production and consumption are accompanied by significant heat losses which generate a direct nuisance on the environment and contribute to climate change. One of the promising routes to new energy resources is the use of this waste heat. In such a context, an interesting way for the direct conversion of low grade heat into electricity is the use of thermogalvanic cells (TGCs) containing ionic liquids (ILs) as electrolyte.1,2

Our choice of the system was focused on the solutions of europium in 1-ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide (EMIM.TFSI). The apparent standard potential of the redox couple Eu(III)/Eu(II) strongly depends on the temperature in various ILs based on the anion TFSI-, our objective was therefore to explain this phenomenon and to develop new TGCs.3 We studied the properties of the solutions of europium(III) and (II) as a function of temperature and in the presence of various ligands (water, dimethylsulfoxide, dimethylacetamide, bromides, etc.) by numerous spectral and electrochemical methods.

Cyclic voltammetry study has shown that electroreduction of europium(III) species is irreversible in an anhydrous medium on a glassy carbon electrode. However, the redox process becomes quasi-reversible after the addition of ligands or the temperature increase. In particular, we studied the competitive complexation of europium(III) ions by water and TFSI- or Br- anions over a wide range of temperatures. The diffusion coefficients of the europium(III) species were of the order of 10-7 cm2.s-1 at 61.5 ° C. In our work, we have shown that the Seebeck coefficient can reach a record value of -5.5 mV.K-1 due to the competitive complexation of europium ions in ionic liquid medium.

The new TGCs were tested under open and closed circuit conditions, and the obtained data were in perfect agreement with the results of cyclic voltammetry. The electrical power measurements were carried out and the optimization work is underway.

Key Words: Ionic liquids, Europium, Heat Energy Conversion

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Abstract ID: 637

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster/Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: Gd3+-doped ZnO:SnO2 nanocomposites; sol-gel; Photocatalytics; BOD and COD

Structural properties and enhanced photocatalytic activity against dyes of ZnO:SnO2 nanocomposites activated by Gd3+ ions

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ABSTRACT

The Gd-doped (0, 0.5, 0.8 and 1.2 at.%) ZnO:SnO2 nanocomposites (coded as G0, G1, G2, and G3) were synthesized via sol-gel method for advance oxidation process (AOP). The composite phases were observed in the XRD pattern and are attributed to the synergistic effects in AOP. The morphology of G0 to G3 was changed from nanorods to nanoflakes covered with Gd3+ ions by increasing the doping concentration of Gd. The average grain size was decreased for samples G0 to G3 on increasing Gd concentration and was confirmed by FE-SEM. The optical bandgap were increased from 3.20 eV to 3.30 eV from G0 to G3. The photocatalytic activity was investigated against the degradation of different dyes for samples from G0 to G3 using different irradiation sources. The sample G2 with optimized loading dose shows highest degradation efficiency for various dyes with different pH aqueous media. The estimation of mineralization factors of dyes were examined through biological oxygen demand (BOD) and chemical oxygen demand (COD) tests before and after AOP. The investigations are very promising for degradation process in rare earth doped metal oxide nanocomposites.

Abstract ID: 638

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Functional Magnetic Materials

Keywords: Magnetorheological gels, Magneto-mechanics, Viscoelasticity, Carbonyl Iron, Size effect

Modeling of Magnetorheolological gels: A Study on the particle size effect

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Magnetorheological Gels (MRGs) belong to a group of advanced multi-functional materials whose properties can be altered upon the application of an external magnetic field. Usually, MRGs consist of micron and/or nano-sized magnetic particles dispersed in a polymeric gel matrix. Few applications of MRGs include vibration isolation devices, adaptive tuned vibration absorbers, and tunable stiffness actuators.

The mechanical response of MRGs arises from the elastic and viscous contribution of magnetic particles and the polymer matrix, while the magnetic response arises from the interaction between the magnetic particles and the applied external field. In the last two decades, various continuum-based models have been developed to predict this magneto-mechanical behavior of MR materials; however, sometimes, they lack detailed information on the arrangement of particles within the polymer matrix. Hence, a microstructural based approach is adopted to develop a model to study the behavior of the MRGs.

The model developed comprises of the elastic contribution related to the magnetic particles and polymer matrix, the viscoelastic contribution related to the creep or relaxation response of the polymer matrix, the magnetic contribution associated with the interaction between the magnetic particles, and the interfacial contribution linked to the interaction between the particles and the polymeric matrix. The proposed magneto-mechanical constitutive framework is consistent with the thermodynamic framework. Further, the strain energies are developed using the microstructural information of the particle arrangements within the MRGs. This model is utilized to study the influence of the particles' size on the magneto-mechanical behavior of the MRGs.

The developed model is calibrated and validated using a set of experimental data. The results indicate an increasing trend in the modulus value as the particle size decreases under the same volume fraction and magnetic field conditions.

Abstract ID: 639
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Recycling and sustainability of composite materials
Keywords: epoxy resin coating, waste limestone powder, adhesive properties

Analysis of the adhesive properties and microstructure of epoxy resin coatings modified with waste limestone powder

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Recently, civil engineering places great emphasis on the sustainable development and recycling of waste materials. The management of waste mineral powders is one of the greatest problems. These powders are derived from the extraction and processing of mineral resources and are nowadays not all re-used, but only stored in heaps. These wastes contains quartz, alumina or limestone fine powders. They are extremely hazardous in this form because they can cause pneumoconiosis, affect the nervous system in animals, pollute water and plants. On the other hand the chemical composition as well as the particle size characteristics make this byproduct an attractive additive to be used in epoxy resin coatings. The addition of waste mineral powders would reduce the total mass of epoxy resins used to make the coatings. However, the research to date on this subject contains many gaps. The epoxy resin is very harmful to the environment, especially to aquatic organisms. The use of the waste mineral powders would make the epoxy resin coatings more eco-friendly. With the above in mind, the main goal of the research was to find an amount of waste limestone powder that would improve or at least not deteriorate the pull-off strength of the epoxy resin coating. This pull-off strength is particularly important for the durability of the coating. The goal of the research was also to analyze the microstructure and chemical composition within the interphase zone between epoxy resin modifies with waste limestone powder and the substrate. The tests were carried out on a 15 cm thick substrate made of C30/37 concrete. The substrate was divided into two areas with different methods of substrates surface treatment (ground surface and patched surface). On both types of the surfaces, five squares were separated for the coatings with the addition of waste limestone powder and one square for the reference sample. Before applying the coating, the morphology of the concrete surface was be examined using a 3D laser scanner. An epoxy resin coating was then applied with a gradually increasing content of the selected waste limestone powder. The reference squares were covered with the epoxy resin coating without waste limestone powder. The measurements of the pull-off strength of the epoxy resin coatings were performed after the coating hardened using the pull-off method according to ASTM D4541. The chemical composition of the material was analyzed in the interface between epoxy resin modified with waste limestone powder and the substrate using a scanning electron microscope and X-ray micro CT. Then, the microstructure of the samples were evaluated using a micro-computed tomography. Analyzing the obtained data in ImageJ and Mathematica, graphs of fractional share of pores along the sample's height of the subsurface zone were obtained. The set goal of the research was achieved by obtaining mechanical properties at a similar level of newly formed epoxy resins.

Abstract ID: 640

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanomaterials and Nanotechnology

Keywords: artificial photosynthesis, nanoparticles, semiconductors, segregation

Better Artificial Photosynthesis by Ion Segregation in Oxide Nanoparticles

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The increase of greenhouse gas in the atmosphere opens an opportunity to use CO2 and water as a raw material for the manufacture of organic molecules by artificial photosynthesis. Among the different approaches to artificial photosynthesis, the use of semiconductor oxides stands out due to the possibility of generating nanoparticles with large surface areas. However, there is a great challenge to develop nanostructures adapted for the reaction in the gaseous phase, since the solubility of CO2 in water is limited. Among the different aspects related to the nanostructure of these materials, the construction of surfaces that allow the simultaneous adsorption of water and carbon dioxide is necessary. At the same time, the nanoparticles must absorb light and generate electron-hole pairs with a sufficient lifetime so that the water oxidation and CO2 reduction can occur satisfactorily. In this case, a large main free path of the electrical charges is important to increase the recombination time that can be improved by increase the conductivity of grain boundaries. Both conditions can be obtained by change the interface composition by segregation of additives during nanoparticles preparation. Segregation is a thermodynamically spontaneous process that modifies the adsorption sites, the depletion layer at the solid-solid interfaces and controls the growth kinetics of the particles. The main propose here is to show how the segregation of additives can be a key factor to prepare semiconductor nanoxides with optimize properties for artificial photosynthesis.

Abstract ID: 641

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Nanocomposites, Zinc oxide, degradation dyes, hydrogen production

Layered hybrid nanocomposites ZnO sensitized with nanoparticles as efficient photocatalysts for degradation of organic dyes and hydrogen production

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Nanocomposite materials based on zinc oxides sensitized with nanoparticles have gained increasing attention for their wide range of potential applications in photocatalysts for degradation of organic dyes and hydrogen production. In this study, efficient photocatalysts based on layered hybrid ZnO nanocomposites with Cu2O, MoS2 and CdTe nanoparticles (NPs) were successfully synthesized and characterized for degradation of organic dyes and hydrogen production. The results provide evidence that layered hybrid ZnO nanocomposites with nanoparticles have the potential to be more efficient photocatalysts for photodegradation of organic dyes and hydrogen production. The improved photocatalytic performance is attributed to the use of hybrid ZnO-carboxylic acid layered materials that have a higher specific surface area and more active sites available, integrating the merits of the superior ability of nanoparticles (NPs) to harvest visible light and to increase the charge separation as well. Furthermore, possible photocatalytic charge carrier migration mechanisms based on alignments of energy band structures and active species capture experiments were proposed. Photocatalytic reuse tests showed that stability and activity were maintained for three cycles

Abstract ID: 642

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Optical properties of metals and non-metals

Keywords: triplet emitters; iridium emitters; organic light-emitting devices; light-emitting electrochemical cells

Hetero-bimetallic phosphorescent IrIII complexes based on carbene scaffolds and their application in light-emitting devices

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Phosphorescent complexes have been extensively investigated in the last few decades in the fields of organometallic chemistry as well as materials science due to their outstanding photophysical and redox properties.[1] Following the seminal work of Thompson and Forrest,[2] great interest in these classes of photoactive compounds has emerged mainly driven by their application as triplet emitters in phosphorescent organic light-emitting diodes (PhOLEDs). where Ir(ppy)3-family of complexes (ppy = cyclometalating phenyl-pyridine type of ligands) often represent emitters of choice.[1] On the other hand, NHCs represent an ubiquitous class of ligands in organometallic chemistry since the discovery of stable NHCs[3] The popularity of NHCs stems from the peculiar combination of unique features such as strong □-donating and relatively weak □-accepting ability and stable M–C bonds, which made them appealing also for designing of phosphorescent emitters.[4]

During the talk, our most recent results in the field will be presented including a novel class of phosphorescent cationic heterobimetallic IrIII/MI complexes, where MI = CuI and AuI where the two metal centers are connected by the hybrid bridging 1,3-dimesityl-5-acetylimidazol-2-ylidene-4-olate (IMesAcac) ligand that combines both a chelating acetylacetonato-like and a monodentate N-heterocyclic carbene site coordinated onto an IrIII and a MI center, respectively. These cationic red-emissive bimetallic species displayed up to two-fold increase of the photoluminescence quantum yield and radiative rate constant compared to the corresponding mononuclear benchmarks,[5] and achieve record PLQY of 65% for cationic organometallic red emitters. Finally, they successful application as electrolumescent materials in light-emitting electrochemical cells (LECs) will be presented.[6]

Key Words: triplet emitters, iridium emitters, organic light-emitting devices, light-emitting electrochemical cells

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Abstract ID: 643

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Processing and manufacturing technologies

Keywords: prosthetic hand, continuum structure, variable stiffness, tendon-driven

Research on the tendon-driven variable stiffness control method for prosthetic hand

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The dexterity of human hands is crucial in completing everyday tasks. The variable stiffness of human fingers is essentially to object manipulation and overall hand dexterity. However, variable stiffness has been overlooked by many extant prosthetic hand designs. Aiming at combining variable stiffness of prosthetic finger to the grasp and hold tasks, this paper presented a variable stiffness control method for prosthetic fingers based on continuum structure only with tendon. With the cooperation of extensor and flexor, fingers can achieve different stiffness in different tasks. According to the bionic inspiration of tendon antagonism of human hand, the proposed method achieved the different/same stiffness combinations at the different/same position by pulling bilateral ropes. The fitting trajectory curve of the finger end position was found by many finger-bending experiments, which is related to the specific parameters of the finger and is the foundation of variable stiffness at the different/same position. By changing the tendon length of active side and passive side, the high and low stiffness could be acquired at the same position and the difference is nearly 50%. Based on the experimental results, a variable stiffness model is established, which achieves the purpose of using different stiffness for different objects. Furthermore, the variable stiffness results of prosthetic fingers are implemented in the prosthetic hand and we assess the capability of the prosthetic hand by grasping tests and variable stiffness tests by performing daily object manipulations including playing piano and grasping and holding daily supplies. It has great potential to be applied for effective, adaptable and safe object grasping and is closer to the human hand.

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Abstract ID: 644

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanomaterials and Nanotechnology

Keywords: Strontium titanate, polar ordering, symmetry breaking, flexoelectricity.

Polar ordering in SrTiO3: from symmetry breaking to new functionalities

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Polar ordering is in high demand in various fields such as sensors, actuators, memories and biomedical devices. However, only non-centrosymmetric materials with a polar axis possess a spontaneous polarization. A promising candidate to investigate the evolution of polar ordering is the perovskite strontium titanate (SrTiO3). Unlike most piezoelectric lead-based materials, SrTiO3 is nontoxic. SrTiO3 receives a lot of attention as a basis for a wide variety of complex oxide electronics. At room temperature, SrTiO3 is paraelectric and possesses an inversion center with an ideal cubic perovskite structure (a = 3.905 Å) and a space group Pm"3"¯m. For the centrosymmetric equilibrium, the SrTiO3 structure is neither ferroelectric nor piezoelectric. Polar order has been introduced by various approaches including external electric fields, defect doping, strain, oxygen isotope exchange etc. Tailoring this polar order would allow for new functionalities in SrTiO3 and enable various additional applications including solid-state batteries or memory devices.[1, 2] Here, we demonstrate the effect of nanoindentations and strain gradients on symmetry breaking and the enhancement of polar order in both bulk and thin film form of SrTiO3 using optical excitation of lattice vibrations by mean of Raman spectroscopy and second harmonic generation at room temperature.[3] The study indicates the ability to enhance flexoelectricity and polar surfaces in SrTiO3 for a possible investigation of strain induced new functionalities in insulator and semi conductor materials using spectroscopy methods.

Abstract ID: 645

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanoparticles, Nanowires, and 3D Structures

Keywords: bimetallic nanoparticles, core-shell nanoparticles, surface segregation, molecular dynamics

General Trends in Core-shell Preferences for Bimetallic Nanoparticles

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Core-shell nanoparticles have gathered much attention of the scientific community owing to their potential applications in various fields including biomedical imaging and catalysis. Predicting core-shell preference1-3 is, however, still largely based on a few experimental observations and limited theorical studies, and hence development of new core-shell nanoparticles is normally built on a trial-and-error approach. Here we present general trends of core-shell preferences for 45 bimetallic nanoparticle systems studied by molecular dynamics (MD) and Monte Carlo (MC) simulations. Simulations were performed using LAMMPS code and the embedded-atom method (EAM) potentials were employed for simulating the interactions between atoms in the bimetallic nanoparticle systems composed of 10 metals; Ag, Cu, Au, Pd, Fe, Co, Ni, Pt, Al, and Mo. In order to quantify the core-shell preference, the MD/MC results were analysed to identify surface atoms using the alpha-shapes method. The core and shell compositions of the preferred equilibrium structures of bimetallic combinations were then used to categorize each combination into one of four different types depending on the level of core-shell tendency: mixed, core-shell, highly segregated core-shell, Janus-like. The categorized MD/MC results were also analysed using principal component analysis (PCA) and linear discriminant analysis (LDA) to determine the primary factors that dictate core-shell tendency. Eight possible factors were considered, and cohesive energy and atomic radius are found to be the two primary factors that have an ‘additive’ effect on the segregation level and core-shell preference in the bimetallic nanoparticles studied. In the majority of the investigated combinations, the element with higher cohesive energy has smaller atomic radius and tend to occupy the core. Highly segregated structures (highly segregated core-shell or Janus-like) are expected to form when both the relative cohesive energy difference is greater than ~ 20 % and the relative atomic radius difference is greater than ~ 4 %. However, when the element with higher cohesive energy has larger atomic radius, the core-shell tendency decreases. The general trend observed in the current study can be used as a guide in nanoparticle synthesis methods in which heat-induced surface segregation phenomena play an essential role, and in predicting the equilibrium structures of bimetallic nanoparticles.

Abstract ID: 646

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Nanoparticles, Nanowires, and 3D Structures

Keywords: core@shell metal@metal-oxide nanoparticles, sintering mechanism, molecular dynamics

Sintering mechanisms of core@shell metal@metal-oxide nanoparticles

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Metal@metal-oxide core@shell nanoparticles (NPs) have recently attracted increasing attention and show great potential for various applications, such as sensing1, photo-catalysis2, and dye-sensitized solar cells3. One prevalent phenomenon involving NPs in various applications is sintering (or coalescence), and it can be advantageous, or undesired. Sintering of NPs has been extensively studied using various computational methods, such as molecular dynamics (MD), investigating sintering of metals, metal-oxides, and bimetallic core@shell NPs. It is generally agreed that the dominating sintering mechanisms are surface diffusion and grain boundary diffusion in crystalline materials4 and viscous flow in amorphous clusters5. However, despite the fast-growing interest, no MD studies of the sintering mechanisms of metal@metal-oxide core@shell NPs have been reporting to date. Here, we present the atomic diffusion behaviours and sintering dynamics of three types of metal@metal-oxide NPs with crystalline metal cores and amorphous oxide shells that are investigated using molecular dynamics based on the ReaxFF potentials. The results show that the coalescence process is similar to reported mechanisms for crystalline nanoparticles. However, atomic trajectory tracing reveals that surface diffusion is highly localized and that it is mostly the surface atoms near the contact region that actively participate in the sintering. In other words, contrary to the common understanding of freely moving high mobility surface atoms, atoms located away from the contact region remain distant during the sintering. We expect the sintering mechanism observed in metal@metal-oxide core@shell NPs here to be highly relevant for small metal nanoclusters as they usually have a thin surface oxide layer.

Abstract ID: 647

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Photonic devices and applications

Keywords: Radiative thermostat, Passive cooling/heating, Zero energy thermoregulation

Self-adaptive radiative thermostat to surrounding temperature variation

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Human beings use tremendous energy to keep cool in summer–current effective cooling, e.g., vapor compression and fluid cooled system consumes around 10% of worldwide energy [1]. This high level of energy consumption accompanies with various problems such as ozone depletion and greenhouse effect. To reduce the environmental burden on Earth, passive radiative cooling method is in the limelight in its eco-friend way of lowering the temperature. However, it is unconscious and sustainable method lasts in winter and causes unwanted cooling. Although few prior studies reported efficient thermoregulation techniques [2,3], most of them uses additional energy or stimulation to change heating and cooling states. Here, we suggest surrounding temperature variant radiative thermostat (STVRT) to realize completely passive way for winter heating and summer cooling. The STVRT changes its cooling and heating states depends on designated temperature points. Our design consists of two core parts: partial solar absorber and thermal radiator within long-wavelength infrared region (LWIR) atmospheric window (i.e., 8-13 μm).

The appropriate solar absorbing portion is strongly needed to achieve winter heating. Based on thermal equilibrium equation, we extort the combination of ~ 14% of solar absorption layer (0.25-2.5 μm-wavelength) with ~ 85% of heat radiation layer (8-13 μm-wavelength). The proposed STVRT can reach +9.6 ℃ heating and –7.4 ℃ of cooling when surrounding temperatures are 0 and 30 ℃ in ideal case (i.e., non-radiative heat exchange coefficient, hc = 0 W/m2/K), respectively. For considering practical case, where hc = 10 W/m2/K, the archived heating temperature is -2.2 ℃ and cooling temperature is +2 ℃ when surrounding temperature is 30 and 0 ℃, respectively. With these intuitive design, we experimentally demonstrate STVRT by coating using porous poly(methyl-methacrylate) (PMMA) (i.e., radiative layer) on Cu film (i.e., absorbing layer). The coating thickness of porous PMMA controls the solar transparency. Also, the material selection can be expanded as long as each layer takes engineered portion of absorption/emission. The design basic shows generalized solution for temperature homeostasis.

Abstract ID: 648

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanoparticles, Nanowires, and 3D Structures

Keywords: Bicontinuous microemulsion, Hierarchical Superstructure, SERS, electrocatalyst

Nano-meso-macro: Synthesis of Hierarchical Superstructures (HSSs) in Bicontinuous Microemulsions for Electrocatalysis and SERS

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Hierarchical superstructures (HSSs) are 3-D structures with a significant improvement in some properties as compared to isolated nanoparticles. However, formation of HSSs has been conducted by intricate methods that usually involve synthesis of the building blocks and the assembly in superstructures in a second step. As alternative one-pot procedure, we propose the use of bicontinuous microemulsions (BCME). The channels of BCMEs have a thickness in the nanometer scale. Both water and oil channels are continuous phases, having infinite lengths. Thus, it is feasible to imagine the growth of HSS inside them, as the narrow thickness of the channels will allow the formation of nanometer building blocks, whilst their interconnection allows for the self-assembly of these nanoparticles into macroscopic 3D networks. The use of BCME for the synthesis of inorganic nanomaterials is rare, in comparison to the use of W/O and O/W ME. When BCME have been used in the literature, isolated and well dispersed NPs has been obtained, mostly using ionic surfactants and water-soluble precursors. In this investigation, we used BCME based on the nonionic system water/ Synperonic 91/5 /isooctane for the synthesis of Pt, PtCo3O4, PtCoNi, PtAu and Ag HSSs. The use of both water- and oil-soluble precursors were compared. HSSs resembling nanocorals, made by interconnected NPs or nanoneedles were obtained (Pt, PtCo3O4, PtCoNi, PtAu), both by chemical reduction and electrodeposition. These materials were explored as electrocatalysts. On the other hand, for Ag superstructures, it was necessary to add a stabilizer (sodium citrate) in order to form a Ag HSS, which was assessed as Surface Enhanced Raman Spectroscopy (SERS) substrate, resulting in analytical enhancement factors in the order of 109 for Rhodamine 6G. These results demonstrate the usefulness of employing certain BCME for HSSs synthesis of, although the concept is not universal to all BCMEs.

Abstract ID: 649
Symposium 4: Functional Composite Materials (FCM)
Poster/Oral Presentation
Topics: Smart Composites
Keywords: 3D Printing, Hydrogel, Smart Materials, Drug delivery

3D Printable Poly(N-isopropyl acrylamide-co-acrylamide) Sodium Alginate Double-network Hydrogels for Dermal Drug Delivery

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Poly(N-isopropyl acrylamide) (PNIPAAm) hydrogels have shown promise for dermal drug delivery, but have been limited by the inferior strength of their swollen state. We report an exploration of using a novel P(N-isopropyl acrylamide-co-Acrylamide) system that combines Sodium Alginate incorporated into the polymer, which significantly improved the hydrogel strength in the collapsed and swollen state while still allowing the temperature dependant swelling of the PNIPAAm based hydrogels. By tailoring the resin formulation for 3D printing, the lower critical solution temperature can be modified leading to printed parts with varying swelling behaviours at multiple temperatures. This study offers a promising method for the fabrication of 3D printable hydrogel structures with mechanical properties similar to cast in place hydrogels. The judicious use of solvents for 3D Printing has enabled us to print out larger parts with little change in the composition of the resin. This study offers a promising method for the fabrication of large customized hydrogel devices that can conform to complex body geometries with the possibility of dermal drug delivery by loading the hydrogel with hydrophilic drugs.

Abstract ID: 650

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Theory of graphene, Mxenes and other two-dimensional materials

Keywords: PdSe2, 2D materials, Nanoelectronics, First-principles modeling

PdSe2: a Pentagonal Layered Material Bridging the Gap Between 2D and 3D Materials

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PdSe2 is a new layered material with an in-plane pentagonal network and stronger-than-vdW interlayer coupling. It offers great trade-off between carrier mobility, band gap, and air stability for nanoelectronics [1]. Because of its unique atomic structure and strong interlayer coupling, it behaves like 2.5D material and many of its properties are different from those of commonly known 2D materials, such as graphene and MoS2. Here I will highlight how first-principles modeling/simulation guided experiments to explore its structural, electronic, and vibrational properties. Because of strong interlayer coupling, its electronic band gap varies significantly from 1.3 eV (monolayer) to 0.06 eV (bulk), based on calculations and measurements [1]. For 2D graphene and MoS2 that have weak interlayer interactions, the layers are quasi-rigid in low-frequency interlayer vibrations, which can be described by a linear chain model (LCM); however, in PdSe2 the layers are no longer quasi-rigid, according to our Raman scattering calculations and measurements. Therefore, the thickness dependence of the interlayer Raman modes' frequencies in PdSe2 deviates significantly from the LCM. A revised LCM was developed to account for the layer non-rigidity [2]. Finally, our calculations found that the pentagonal structure and strong interlayer coupling lead to low diffusion energy barriers for defects, and hence both intralayer and interlayer hopping of defects can occur relatively easily in PdSe2 compared to MoS2, as observed by scanning tunneling microscope (STM) [3]. Interestingly, the high mobility of defects and strong interlayer coupling in PdSe2 also contribute to phase transition to multiple different structures: including 2D Pd2Se2, 3D Pd2Se2, and 1D pentagonal PdSe2 nanoribbons, as corroborated by our DFT calculations and the atomic-scale STM simulations [4]. Our joint theoretical/experimental works demonstrate that PdSe2 is a novel layered material featuring great transistor performance, strong interlayer coupling, versatile phase transition, etc.

Abstract ID: 651
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Multifunctional composites
Keywords: nanocarriers, bacteriabots, targeted delivery, antimicrobial actives

Bacteriabots - motile "stealth" biological carriers of novel nano-antimicrobial actives

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The spread of antimicrobial resistant bacteria (e.g. Staphylococcus aureus and Pseudomonas aeruginosa) is a global healthcare concern, reflected in poor treatment outcomes, leading to serious clinical complications, increased mortality, and huge financial burden. During the infection establishment, bacterial cell-to-cell communication process, called quorum sensing (QS), regulates the virulence factors production and formation of antibiotic resistant biofilms via the secretion of highly specific signal molecules. We present a novel micro-transportation system, Bacteriabots, for faster and targeted delivery of antimicrobial actives directly to the site of infection.

These nano-vehicles are composed by a non-pathogenic motile bacteria (carrier) loaded with a nano-enabled cargo entity (e.g. nanoparticles, nanogels) that shows high selective bactericidal efficacy towards Gram positive or Gram negative strains. Our approach would take advantage of the swimming capabilities of non-pathogenic motile human microbiome bacteria. Chemical bonding or electrostatic interactions between the biological carrier and the nano-formulated bactericides will lead to effective formation of the new biohybrid micro-transportation system, in which Bacteriabots driven by Gram positive bacteria will carry the targeted actives against P. aeruginosa and Gram negative carriers against S. aureus. The appropriate cargo and carrier characterization in addition to antimicrobial assays will be presented.

Abstract ID: 652

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Electrical, optical, electrochemical, thermal and mechanical properties of graphene, Mxenes and other two-dimensional materials

Keywords: CQD, Photoluminescence, HR-TEM, Optical Absorption, Functional Groups

Morphology, Absorption and Emission Study in Carbon Quantum Dots Synthesized by an Electrochemical Top-Down Method.

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Carbon quantum dots with different sizes have been synthesized by an electrochemical Top-Down method, its surface was passivated with ethylene glycol. The effect of interaction between quantum confinement, morphology and carbon functional groups, was investigated by means of the High-Resolution Transmission Electron Microscopy (HRTEM), Optical Absorption Spectroscopy, (OAS) and Photoluminescence Spectroscopy (PL). HRTEM experiments have been applied to study of morphology, the resultant CQDs were relatively short (having diameters of 2-7 nm), however study of Optical Absorption gave rise to a defined absorption peak in the visible spectral region, this is result could be explained due uniform sizes. PL of Synthesized CQD were studied at room temperature, PL bands obtained are related to the quantum confinement process and the interactions with the different functional groups. In the present study, the tuning of PL emission is shown and studied in a range from 400 nm to 800 nm. In the same way, the study of PL was carried out in a temperature range 10K to 300K, studying the activation energies, peculiarities of HRTEM, OAS and PL are analyzed and discussed.

Abstract ID: 653

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Electrical, optical, electrochemical, thermal and mechanical properties of graphene, Mxenes and other two-dimensional materials

Keywords: MXenes, Titanium Carbide, Biological Buffers, Amines

Molecular Interactions Between Ti3C2 MXene and Amine Containing Molecules in Aqueous Buffered Solutions

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MXenes, a family of ultrathin layered two-dimensional (2D) transition metal carbides, nitrides, and carbonitrides are steadily advancing as novel inorganic nanosystems for various electronic applications. While the metallic conductivity, solution processability, hydrophilic nature, and presence of various surface functional groups enable the use of 2D MXenes in aqueous systems possible, studies aiming to use MXenes in aqueous and especially biological systems are limited. We investigated the structural and functional properties of Ti3C2Tx (T = F, OH) MXenes in N-substituted biological buffers like N-(2-Hydroxyethyl)-piperazine-N'-ethanesulfonic acid (HEPES) and 3-(N-morpholino)-propane sulfonic acid (MOPS) and with a series of amine-containing small molecules when dissolved in phosphate buffer solution. UV-Vis measurements of MXenes when dissolved in solution reveal a striking impact on their absorption spectra in the presence of amine-containing molecules. XRD and electrical conductivity measurements of MXene films which were exposed to amine containing molecules clearly show that these molecules intercalate between MXene nanosheets and significantly affect their electrical conductivity. The interactions of Ti3C2Tx MXenes with amine-containing molecules is structure-dependent and are fully reversible. This suggests the interactions are driven by weak bonding interactions like hydrogen bonding and/or electrostatic interactions. This study is an important step toward understanding the stability of MXenes in aqueous media, and the ability to predict the interactions of MXenes and small amine-containing molecules and later larger biomolecules. The reversible nature of the interactions between MXenes and small amine-containing molecules, revealed in our study, open new possibilities for the development of MXenes containing chemical sensing thin films for use in aqueous media.

Abstract ID: 654

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Nanostructured materials for advanced batteries
Keywords: Band tails, Fermi function; extrinsic n-type semiconductors.

Student understanding of Fermi energy, the Fermi-Dirac distribution Statistics for deeply doped n-type semiconductors

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Attempts are made to the study of the Fermi-function of the experienced semiconductor by forming a band currencies opposite side on the basis of newly introduce legislation electron scattering.Untideiness screening possibility of a particular value for and with the Fermi-Dirac function relative changes begin at the zero value of the land and the growing electronic power with the decrease is .The speed with magnification growth occurs , and the superior quality for , approach. Subsequently showing the smallest value, the increases at a moderately slow rate with cumulative energy and for developed value energy , lines to . The current formula in its decline, falling semiconductor transporting property to search for the key symptoms , and that's as a result , Boltzmann transport equation solution on rely on and experiment with the more well agree to be expected that .

Abstract ID: 655

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Chitosan, Composite, Beads, Polymerized ionic liquids, Biopolymers

Evaluation of Polymeric Ionic Liquids-Chitosan Beads as An Innovative Adsorbent to Trace Multitarget Analytes from Waste water

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Pyridine based polymerized ionic liquids were successfully utilized for the first time with the combination of chitosan (Cs) and graphene oxide (GO) as an innovative adsorbent to trace multitarget analytes from waste water. A very simple and easy system (peristaltic pump) was exploited to produce sphere-shaped minor and fine beads. Consequently, the following three samples were prepared and characterized: Cs-beads, poly (4-vinylpyridine) octyl bromide/Cs-beads, poly (4-vinylpyridine) octyl bromide/Cs/GO-beads. Infrared Spectroscopy (IR) confirmed the chemical connections present among all constituents. Scanning Electron Microscopy (SEM) revealed the porous nature of adsorbent. Beads was tried for the elimination of heavy metals and organic pollutants from waste water. Arsenic and copper ions were designated as model pollutants to address heavy metals, methylene blue and naphthalene were also carefully chosen pollutants to report organic family. Batch adsorption technique was used. Inductive Coupled Plasma-Optical Emission Spectroscopy (ICP-OES) was used for the analysis of the remaining quantity of arsenic metal, copper ions were detected through atomic absorption spectroscopy. UV-visible spectroscopy and high-performance liquid chromatography were used to analyzed dye and naphthalene uptake, respectively. Polymeric ionic liquids-based composites beads showed good adsorption behavior towards metal ions. The adsorption capacity of beads towards copper ions uptake was around 98 %. The chosen adsorbent was poly (4-vinyl pyridine) octyl bromide/Cs/GO-beads. The results encourage the integration of poly (4-vinyl pyridine) octyl bromide with other polymers and fillers for further improvement in related applications.

Abstract ID: 656

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Porous and cellular materials

Keywords: Cell-on-chip, Microfluidics, Drug toxicity testing, 3D cell culturing, porous membrane

A cost-effective microfluidic cell-on-chip platform for HepG2 cell using porous polymer membrane

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Microfluidic 3D cell culture platforms are essentially microfluidic channels that support three-dimensional cell growth. As opposed to the conventional cell cultures in Petri dishes, microfluidic cell cultures offer the advantage of reproducing a 3D in-vivo like microenvironment. These cell-on-chip devices are a step closer to developing more efficient organ-on-chip devices that have the promise to revamp the existing drug development pipeline by eliminating animal testing, accelerating the process, and prevent clinical trial volunteers from life-threatening side effects in case of drug failure. We have designed a simple microfluidic cell-on-chip device to culture liver hepatocellular carcinoma (HepG2) cells through a customized photolithography process. Polydimethylsiloxane (PDMS) has been used to fabricate this device. The device supports HepG2 cell viability as evident from the cell viability assay, MTT. In order to check the effect of the substrate on cell adhesion and growth, we cast the device on various polymer substrates like polystyrene, PDMS, polyvinylidene fluoride (PVDF), nitrocellulose, and glass. In addition to this, the cytotoxicity of nanosilver at varying concentrations was visualized using MTT assay and PI staining. One of the advantages of this cell-on-chip platform is that it can be easily multiplexed and adapted to culture other cell types by making minor changes in the design.

Abstract ID: 657

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Nanomaterials and Nanotechnology

Keywords: Electrical Breakdown, Charge transport, TiO2 nanotubes, Morphology, Electrolyte

Charge transport and electrical breakdown in single TiO2 nanotubes depending on morphology

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Understanding the electrical conduction properties of a single nanostructure is important for an insight into the fundamental charge transport through the one-dimensional materials and also for exploring the collective behavior of an array of such nanostructures. TiO2 nanostructures, such as electrochemically grown nanotubes, have been widely studied in recent times for several applications. The electrolyte plays a vital role in deciding the morphology, which, in turn, govern charge transport behavior. Here we present a comparative study of the charge transport through a single TiO2 nanotube grown by electrochemical anodization using Ethylene Glycol (EGTNT) and Dimethyl Sulphoxide electrolytes (DMTNT). The individual nanotubes are assembled into nanodevices using photolithography without relying on complex and sophisticated processes like electron beam lithography or focused ion beam deposition. The electric field dependent charge transport properties show Schottky emission at lower field regime and Poole-Frenkel emission in the higher region and the dielectric constant 32.78 (EGTNT) and 7.34 (DMTNT) of two types of nanotubes has been derived from the fitting parameters. The temperature-dependent electrical conduction (110K - 410K) is mediated by two thermal activation processes, attributed to shallow impurities in the low-temperature range ($T < 230$ K) and to the donors at deep intermediate levels at higher temperatures ($T > 230$ K). The shallow and deep donor density has been estimated from the fitting parameters of the Arrhenius equation. The activation energies for EG based nanotubes (122 ± 5 meV) are found to be higher than that of DMSO nanotubes (115 ± 4 meV) owing to the doubled wall morphology of the formed tubes. Also, the study of the electrical breakdown phenomena of these nanotubes reveals three distinct categories of collapse. ‘Model I’ type breakdown is characterized by a stepwise rise of current up to the breakdown point and fall to zero following a non-uniform step by step decrement, which is driven by crack formation near the electrode interface and it’s propagation. ‘Model II’ shows a transient rise and fall in current, leading to breakdown due to electromigration. Whereas ‘Model III’ type breakdown observed in a bundle of nanotubes shows a mixed trend of ‘Model I’ and ‘Model II.’ The data and analysis provide insight into the current limit through an individual nanotube or bundle of nanotubes and will be useful for designing prototype nanodevices from titania nanostructures.

Abstract ID: 658

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Polymeric composites

Keywords: Humidity, Nanocomposite, Sensor

Humidity sensor based on Poly(lactic acid)/PANI-ZnO composite

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The detection and monitoring of humidity are of great importance in many fields, such as textile, agriculture, medicine, and electronics [1]. An ideal humidity sensing material usually has good sensitivity, quick response, and quick recovery time. We have synthesized a polymer nanocomposite-based humidity sensing material, in which we have used an electrospinning technique to prepare the micro-fibers of PLA/PANI-ZnO composite. The PANI/ZnO nanocomposites are synthesized by hydrothermal and in-situ polymerization methods. The X-ray diffraction technique is used to study the structural properties of the PLA/PANI-ZnO composite fibers and PANI-ZnO nanocomposite. In this experiment, the average crystallite size of the PANI-ZnO nanocomposite is found to be 36 nm. The morphology of the composite fibers is analyzed by a scanning electron microscopy (SEM). The average fiber diameter of the pure PLA and PLA/PANI-ZnO composite fiber are ~2.5 µm and ~1.4 µm, respectively. Differential scanning calorimetry (DSC) provides the thermal properties of the PLA/PANI-ZnO composite fibers. The melting temperature (Tm) for the pure PLA is observed at 149.3 °C, and is shifted to 153.0 °C for the PLA/PANI-ZnO composite fibers. The enhanced thermal properties of the composite fibers are due to the interaction between the polymer and the nanoparticles. The water contact angle measurements probe the surface hydrophilicity of the PLA/PANI-ZnO composite fibers. We have also investigated the role of PANI-ZnO nanocomposite on the sensing behavior of PLA fibers. The humidity sensing properties of the composite fiber sensor are also studied in the relative humidity (RH) range of 20-90 % RH. The experimental results show that the composite fiber exhibits good response (85 s) and recovery (120 s) time. These results indicate that the one-dimensional fiber structure enhances the humidity sensing properties.

Abstract ID: 659

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanoparticles, Nanowires, and 3D Structures

Keywords: Nanostructures, Electron-phonon Coupling, Resonant Raman Scattering, Huang-Rhys Factor

Electron-phonon coupling in semiconductor nanostructures: intrinsic and extrinsic tunability demonstrated with ZnTe nanowires

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The dependence of electron-phonon coupling (EPC) on nanostructure size has been a topic of controversial over three decades. Often, the EPC was probed by resonant Raman scattering (RRS) using the 2LO to 1LO intensity ratio R21 to extract the Huang-Rhys factor [1] (S) by applying Albrecht's theory,[2] where the bulk reference S was calculated by using a theoretical model developed for a bound exciton with Fröhlich interaction.[3] The issue involves multiple aspects: (1) What would be the appropriate mechanism for the nLO Raman lines in the bulk material, since they already exist in the bulk material and are only modified in the nanostructures? (2) What does R21 tell about EPC? (3) Were the observed changes of intrinsic to the nanostructures? We note that the S factor and Albrecht's theory both are based on lattice relaxation that typically occurs when a highly localized state is involved in an optical transition. Thus, they do not apply to the nLO in RRS in bulk and likely to most cases of the nanostructures.[4] Since R21 has been found to be very large (because 1LO is very weak) in high quality bulk materials, decrease in R21 actually implies increase in EPC for the specific process rather weakening in EPC as often suggested.[5] We have shown [6] that in ZnTe, in contrast to the previous reports, R21 exhibits a much larger intrinsic value and minimal change from bulk to 30 nm nanowire, indicating previously reported size dependences were likely affected by extrinsic mechanisms. In fact, the ratio can be tuned extrinsically over one order in magnitude controllably either during or post growth, allowing for programing EPC in nanoscale devices. Similar degree of tunability has also been demonstrated in ZnTe thin-film samples. This work provides unambiguous experimental results for developing EPC theories for reduced dimensionality and defect influence, and suggests the need to reexamine the reported results for different material systems to distinguish the intrinsic and extrinsic effects.

Key Words: Nanostructures, Electron-phonon Coupling, Resonant Raman Scattering

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Abstract ID: 660

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Anodes and cathodes Materials

Keywords: Battery, Cathode Materials, Redox Mechanism, Soft X-ray Spectroscopy, Oxygen Redox Reaction

Cationic and Anionic Redox Chemistry in Oxide-Based Battery Cathodes

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The pressing demand of high energy batteries for modern energy applications calls for clarifications and optimizations of the redox chemistry involved in battery operations. As the bottleneck of battery energy density, oxide-based battery cathodes suffer complicated issues of the involvements of both the transition metal (cation) and the oxygen (anion) in the redox reactions during the high voltage cycling, which relies on modern characterization tools to reveal the underlying chemistry and guidelines for optimizations.

This presentation introduces recent developments and studies of oxide cathodes through advanced soft X-ray spectroscopy, especially resonant inelastic X-ray scattering (RIXS) in the soft X-ray range of the oxygen (K-edge) and transition metals (L-edges)[1]. We discuss several demonstrations on Li-ion and Na-ion battery cathode studies[2], and provide our spectroscopic views on the TM and Oxygen redox behaviors in Li-rich and conventional cathode compounds[3], which are directly related with some critical issues, such as stability[4] and kinetics[5], in batteries operated at high voltages.

Key Words: Battery, Cathode Materials, Redox Mechanism, Soft X-ray Spectroscopy, Oxygen Redox Reaction

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Abstract ID: 661
Symposium 4: Functional Composite Materials (FCM)
Poster/Oral Presentation
Topics: Green Composites
Keywords: Sustainable Production, Powder Technology, Construction Materials

Production of Green Cementitious Composites: Granite Powder Utilization

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Nowadays, CO2 emissions to the atmosphere have been growing steadily for several decades. Environmental protection has become one of the priority tasks of scientists from around the world. Researchers are trying to find ways to produce the most important materials that way, to reduce CO2 emissions to the atmosphere. Cement is one of them. Cement production is one of the most adverse CO2 emissions in the world (ca. 8% CO2 emission in the world). Looking for opportunities to improve the natural environment, we should look for alternative material solutions (for example marble and limestone powders). Now, researchers are trying to reduce the amount of cement in cementitious mixes by replacing it with supplementary cementitious materials (SCM's). One of the most commonly used SCM in cementitious mixes are mineral powders (f.e. granite powder waste).

Granite powder waste is a waste material generated by crushing granite rocks or cutting granite rocks. So far, that material has been treated as waste, but the search for new SCM's caused, that it is increasingly used to reduce the amount of cement in cementitious mixes.

The main aim of the article is to determine the possibility of reducing the environmental footprint of cementitious composites produced with the use of granite powder waste. Comparative research were carried out related to the subject of fresh and hardened properties of cement mortars with the addition of granite powder waste. Based on the performed research, the main properties related to the utilization of GP in cement mortars are described. Additionally, the problems related to the preparation of this waste for use in the production of cements and cement mixtures were described. In order to determine the possibility of using granite powder waste in cementitious mixes, the results of the research carried out by the author and the results of other authors available in the literature were compared. The summary indicates the possible use of this waste to sustainable production of building materials.

Abstract ID: 662

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Bio-inspired design of composites

Keywords: bio-inspired, polymer nanocomposite, thermal management, dynamic heat flux control

First-Principles Calculations of the Energy Flux for Bioinspired Personalized Thermal Comfort Wearables

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Thermal management is important for modern technologies - buildings, electronics, and clothing. The animal kingdom offers inspiration for development of materials with excellent thermal management, such as the mirror comb-footed spider (Thwaitesia sp.). The fast dynamic optical color changing capabilities of organelles found on the abdomen of this spider has provided inspiration for new polymer nanocomposite materials with application in thermal management. The developed materials replicate the capability of aforementioned spiders to change the reflectance and transmittance of light in the infrared wavelength range. The nanocomposite materials are safe for human use and are scalable for large-scale application.

The new polymer materials bring together the advantages of passive thermal control (low cost, easily scalable implementation, and efficiency in terms of on/off switching ratio), with on-demand control of temperature specific for active thermal control for unparalleled thermal management. The procedure (Figure 1) can be scaled up with well-known methods for polymer film formation. Our team used the versatile chemistry of silicone and styrene polymers for preparation of films that can manage up to 60 W/m2. This capability for managing the thermal flux can be tuned in real time by mechanical or electrical actuation, with an input of <5 W/m2. Inside office buildings ~60% of the heat exchange between the human body and the environment takes place through infrared radiation, and the nanocomposite materials in unactuated state can reflect infrared radiation as well as the space blanket developed by NASA in 1960. By mimicking the change in surface area of the plates on the spiders' abdomen, the nanocomposites can modulate up to 70% of the heat flux emitted by the human body. With introduction of such materials in clothing, the thermal comfort range can be expanded, leading to ~3% energy savings of global commercial energy consumption.

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Abstract ID: 663
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Green Composites
Keywords: Deep Eutectic Solvents, Thin Film Microextraction

Application of new SPME sorbent materials modified by deep eutectic solvents for preconcentration of trace amounts of organic contaminants in environmental sample analysis

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Nowadays targets in analytical chemistry include the monitoring and assessment of the state of the environment and the determination of trace amounts of contaminants, often in variable and complex matrices. Therefore, it is important to introduce solutions in both the measuring equipment and analytical procedures in accordance with the principles of green analytical chemistry. These principles assume shorter time and less laborious of the analytical procedure, automation and miniaturization of measuring devices, as well as the elimination or reduction of volatile organic compounds, and the reduction of waste.

Therefore, the technique of solid-phase microextraction (SPME) proposed by Arthur and Pawliszyn in 1990 is so popular among scientists. In the SPME technique, analytes are absorbed on a fiber coated with an appropriate sorbent materials. From the point of view of green analytical chemistry, the solvent-free nature of adsorption, as well as the use of little or no solvent in the desorption stage and the possibility of multiple use of the fiber are important.

Currently, the SPME technique is developing mainly towards the composition of new sorbent materials as well as various geometries of fibers [1]. The sorbent materials can also be applied to a flat surface, e.g. as a thin film on a stainless steel mesh that acts as a fiber in an SPME. This related technique is known as thin film microextraction (TFME).

The main assumption of the research is the creation of new sorbent materials modified by deep eutectic solvents and their application for TFME technique.

The range of research includes the design and then synthesis of a large group of new deep eutectic solvents (DESs), and natural deep eutectic solvents (NADESs) in various molar ratios of hydrogen bond donor (HBD) to hydrogen bond acceptor (HBA), which is carried out taking into account their selective use for the extraction of analytes with defined polarity. Next, stable sorbent materials with a high sorption surface were prepared, which obtained by cross-linking DESs / NADESs with a commercial prepolymer and applying them in the form of a thin film to a stainless steel mesh. The TFME technique with new sorbent materials was used to isolation and preconcentration trace amounts of organic analytes followed by their chromatographic analysis.

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Abstract ID: 664
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Multifunctional composites
Keywords: Carbon nanotubes, 3-D hierarchical aerogel, Multifunctional, p-Dicyclopentadiene

Carbon Nanotube Sheets in Advanced Multifunctional Composites

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Due to their outstanding mechanical, electrical and thermal properties, as well as a large aspect ratio and high specific surface areas, carbon nanotubes (CNTs) have been investigated for developing high-performance multifunctional composites. This class of new-generation materials has shown revolutionary impacts not only in academic communities but in industrial fields as well. Here, we report novel methods to fabricate multi-functional CNT composite sheets for a diverse range of applications, including but not limited to aerospace, energy, electronics, electrochemistry, supercapacitors, EMI shielding, and chemical and biosensors.

High strength CNT composite sheets with aligned CNTs, reduced waviness, and consolidated by stretching, poly-dicyclopentadiene (p-DCPD) infiltration, mechanical rolling and polymerization are presented [1]. It is found that the as-produced p-DCPD CNT composite sheets show a tensile strength, Young's modulus, and toughness of 700 MPa, 35 GPa, and 70 MJ·m-3, respectively, which are an order of magnitude higher than the sheets consolidated with solvent (Fig.1a). This enhancement is attributed to the higher load transfer between CNTs and DCPD in the composites. Highly conductive multilayered CNT sheets for EMI shielding have been fabricated by chemical doping with KAuBr4 and mechanical densification as well.

The conductivity of the CNT sheets has been increased from ~1.0 × 104 S/m to over 1.0 × 106 S/m, two orders of magnitude higher. The EMI shielding effectiveness of the gold doped CNT sheet varies from 60 dB to 100 dB in the frequency range from 100 MHz to 18 GHz. Finally, a novel facile and fast method to expand commercial CNT sheets into an ultralight 3-dimensional (3-D) hierarchical aerogel with controllable density, architecture, geometry, pattern, and properties is presented (Fig.1b). The as-produced 3-D CNT aerogels show a hierarchical structure of ultrathin intermingled CNT films with remarkable multifunctionalities, such as low thermal conductivity (40 mW·m−1·K−1), low density (0.9 mg·cm-3), high compressive strength (> 7 kPa), high electrical conductivity (> 100 S·m-1), and high toughness (>3 kJ·m-3).

Abstract ID: 665

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Sensors and MEMS: Materials and Devices

Keywords: Chalcogenide glass, Ag diffusion, UV radiation, Additive manufacturing.

Studies and Performance evaluation of Printed UV Radiation sensor

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This work's primary focus is to fabricate a Ge-Se-based Chalcogenide glass (ChG) printed reversible radiation sensor using additive manufacturing technology. The radiation sensor perofromance relies on Ag ions diffusion within the ChG triggered by the UV irradiation. This causes changes in the ChG material's conductivity, which is measured between two electrodes deposited on the ChG. We have developed a dissolution-based ChG inks formulation process, printed thin films with these inks applying nScrypt & screen printer, and optimized the sintering condition. The dissolution-based Ge-Se ChG inks containing various compositions of both elements were characterized by their viscosity and surface tension. We studied compositional, structural, and surface roughness changes of printed ChG films at different UV radiation doses using Energy Dispersive X-ray Spectroscopy (EDS), Raman Spectroscopy, and Atomic force microscope. These methods also gave data about the interaction of the diffusing Ag ions with the ChG film. The diffusion binary and ternary byproducts, their crystal size, and compositional changes after irradiation were revealed by X-ray diffraction (XRD), Energy Dispersive X-ray Spectroscopy (EDS). The electrical conductivity between the two electrodes was measured using a semiconductor parameter analyzer in a probe station at different irradiation doses. The results show strong evidence of printed dissolution-based ChG inks' functionality, enabling a new research area of Additive manufacturing.

Abstract ID: 666

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Zinc hydroxide, Dyes Encapsulation, Adsorption, Photocatalysis

Zinc Hydroxide Layered Hybrid Supramolecular Structures. Adsorption and Photocatalysis of Dyes

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Hybrid lamellar nanocomposites in which the photophysical properties of broadband oxides such as TiO2 or ZnO are conjugated with the properties of long chain amphiphiles such as amines or carboxylic acids, exhibit superior dye degradation photocatalytic behaviors to those of pristine oxides. The increased catalytic activity of such nanocomposites is due to both the extreme aspect ratio of the inorganic component and the unusually large surface area rich in defects, but also hydrophobic interactions between the dye and the catalyst. In these cases, as in the majority of materials used for the removal or photodegradation of dyes, the catalyst / dye interaction consists of a superficial physisorption, different from the process observed in the case of a new basic laminar zinc hydroxide modified with stearic acid (BLZH-SA). Bulk BLZH-SA can be described as a stack of sheets each formed by a double layer of hydrozincite (Zn5(OH)6(CO3)2) partially substituted by stearate groups, generating a supramolecular entity that defines a network of monomodal pore size (3-4 nm) capable of encapsulating the dye molecule, deciding its adsorption / degradation process. For example, in the dark, BLZH-SA preferentially absorbs anionic dyes (Congo Red, CR, >> Methylene Blue, MB), while under irradiation, either UV or vis, it degrades the dye -CR or MB- in two stages, first the non-adsorbed dye (solution) and then the adsorbed dye (solid). The results are interesting from a practical and fundamental point of view. The possibility of performing both processes - dye absorption in the dark and driven degradation in sunlight - temporarily and locally separated could be useful for applications. Mechanically, these systems are particularly challenging under visible light because they behave as a complex combination of the action of dye-sensitized semiconductors and the self-photodegradation of dye-assisted semiconductor.

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Abstract ID: 667

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanomaterials and Nanotechnology

Keywords: Nanowire, Optical Response, Resistance Switching, Memristor, ZnO

Experimental Observation and Theoretical Modelling of Light Activated Resistance Switching in Single ZnO Nanowire

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Semiconductor nanowires are the building blocks of many nanoscale electrical and neuromorphic circuits. Here, we demonstrate a simple arrangement wherein an ethanol-adsorbed ZnO single nanowire, deposited between gold electrodes using dielectrophoresis exhibits significant change in resistance when activated by visible light. We have observed that the transition timescale between two stable ohmic states, one in the dark and the other in the illuminated regime in a single nanowire can occur in the sub millisecond order, which is 7 orders of magnitude lower than previously reported switching timescale in bulk ZnO thin films. We also demonstrate that visible light acts as a non-invasive tuning parameter for the bistable resistive states that can be potentially used as memory switches in synaptic circuits. A mathematical model of the light activated resistance switching mechanism is proposed based on the adsorption-desorption kinetics of oxygen molecules at the surface of the nanowires, which shows promising agreement between theory and experimental results.

Abstract ID: 668
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Bio-composites
Keywords: Nucleic Acid Nanotechnology, Soft Materials, Sensors

Dynamic self-assembly of compartmentalized DNA nanostructures

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A longstanding challenge in biomaterials science is the development of active materials that can replace or supplement structures or functions present inside biological cells (1). The dynamic cellular cytoskeleton promotes shape changes required for processes such as division, growth, and morphogenesis, but remains difficult to introduce to synthetic systems due to its structural complexity and stringent reconstitution protocols. Nucleic acid (NA) nanotechnology offers a route towards the synthesis of custom, dynamic, micron-scale materials and molecular circuits through hierarchical assembly processes (2,3). However, it remains an open question how such circuits and structures may be synergistically encapsulated and employed inside synthetic cells. We demonstrate the bottom up synthesis of adaptive NA scaffolds in water-in-oil droplets as minimal cell-like compartments. Through different encapsulation methods, we show that micrometer-sized scaffolds assemble under physiological conditions from nanometer-sized, rationally designed precursors. To monitor the dynamics of nanotube polymerization in a large number of compartments, we devise a simple method that takes advantage of statistical properties of the droplet images. Further, by implementing a nanotube design whose formation is fueled by RNA molecules, we achieve nanostructure assembly and disassembly by producing and degrading RNA inside droplets. We further calibrate these chemical reactions and components to obtain transient nanotube assembly, with the possibility of tuning the density of assembled nanotubes as well as for how long they are present in the droplets. We also include light actionable NA sensors to regulate nanotube growth by controlling the nanotube nucleation and polymerization process. Because NA nanotechnology is rapidly expanding, our encapsulated nanotubes may be modularly coupled with a variety of components to achieve more complex biochemical circuits that can fuel autonomous nanotube behaviors in confinement. Thus, our work opens many routes towards achieving dynamic control over the internal organization and the mechanical properties of protocells.

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Abstract ID: 669

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Photonic devices and applications

Keywords: hot carriers, hot electrons, plasmonics, thin films, solar cells, photodetectors

Novel optical materials and structures for hot electron devices

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Metals are used for a variety of electronic components, and the field of plasmonics has expanded their use to optical structures when lowed low-loss metals are implemented. The emerging field of hot electron devices has merged these fields (electronic devices and optics) further. In this presentation, we will discuss our recent work building hot electron photodetectors for NIR detection using Si and metal oxides, improved response using nanoscale metal alloys, and time-resolved ultrafast detection via pump-probe techniques exploiting surface plasmon excitation. Further, we will show how the incorporation of index near zero (INZ) substrates can lead to nearly 100% absorption in thin metal films, providing a new platform for hot electron devices. We will conclude with an outlook and discuss future possibilities with these novel material systems.

Abstract ID: 670

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Electrochemical Supercapacitors

Keywords: Laser scribed, graphene supercapacitors, fractal

Laser Scribed Fractal Graphene Capacitors: Scaling Behavior with Respect to Fractal Order and Complexity

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In past decades, the application of fractals to electrode design for enhanced signaling and electrochemical performance was a popular subject and enabled the growth of consumer micro-electronics. Supercapacitors, which are energy storage devices with many promising characteristics, have largely grown alongside of such developments in electronics, but little work has been done to use fractal electrodes in supercapacitors. In this work, plane-filling and fractal patterns were used in designing laser scribed graphene supercapacitor electrodes, allowing the scaling laws of capacitance with respect to fractal order and complexity to be examined for the first time. An interesting exponential relationship between capacitance and fractal order for the more open structured fractals was observed, the exponent of which was proportional to the Hausdorff dimension. This indicates that two or more competing parameters are at play, likely path resistance and surface area. These results indicate that there is a benefit in using fractal electrodes in supercapacitors, but the magnitude of the benefit depends on the interactions between path length and surface area, and therefore fractal order.

Abstract ID: 671

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Sensors and MEMS: Materials and Devices

Keywords: Multi-responsive Hydrogel Sensors, Microneedle electrochemical probes, Biomimetric Redox Responsive Composite Hydrogels, Industry 4.0 and IoT Devices.

Multiplexed multi-responsive microneedle hydrogel sensors for chemical analytics useful in diverse applications in Industry 4.0

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Chemical sensors are a major segment of Internet of Things (IoT) devices that are key drivers to the emerging fourth industry revolution (industry 4.0)—that broadly speaking aims to create 'self aware' seamlessly interconnected sustainable production ecosystems.

Our research group is focused on developing multi-architecture spectroelectrochemical sensors based on multi-responsive polymers as molecular receptors for multiplex analytes detection. Fabricated by layer by layer (LbL) assembly, in this presentation we will demonstrate our versatile flexible and rigid microneedle electrochemical probes based on biomimetric redox responsive composite hydrogels for in-situ multiplex detection of biologically relevant chemical markers, e.g., dissolved oxygen, redox biomarkers, antioxidants, soil nutrients such as phosphates and nitrates, lactic acid, cortisol, adrenaline, electrolytes, and pH. The composite hydrogels in these sensors simultaneously serves as an interface for biological fluid sampling and a medium for electrochemical sensing. These sensors will be demonstrated as wearable devices, also referred to e-skins, for real-time wireless monitoring of soil/plant growing medium, on-plant plant stress diagnostics, and 'emotion' sensing in animals using non-invasive biological fluids, e.g., sweat, and interstitial fluids for animals, and apoplastic exudates for plants. Our embedded multiplex sensors are aimed to be enabling proactive diagnostics technology for realization of environmental, social and economic aspects that align with the United Nation's Sustainable Development Goals (UN SGDs), particularly sustainable smart agriculture, food security, environmental conservation, and in general equity in global societies wellbeing.

Abstract ID: 672
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Multifunctional composites
Keywords: Bismuth, nanoclusters, layered materials, environmental remediation

Bismuth clusters form nanomaterials for environmental remediation

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Bismuth (Bi) is a heavy element with intriguing properties and, unlike its neighboring lead, antimony, and polonium in the Periodic table, it is neither toxic nor radioactive. It coordinates a wide variety of inorganic and organic ligands, forming structurally diverse complexes in part due to the presence of a stereochemically active pair of 6s electrons, and oxidations states ranging from 0 to +5. Because of their antibacterial properties, Bi-based compounds have been historically studied for medical purposes and found only limited use in other applications, such as cosmetics, pigments, and alloys. Recent realization of unique physicochemical properties related to high diamagnetism, electrical resistivity, catalytic and optical activities, tunable bandgap and others has motivated an upsurge of interest in Bi-based layered nanomaterials. During last two decades, significant progress has been achieved in their rational design and synthesis to attain targeted structures and morphologies. Despite these developments, functional characterization of polycationic oxyhydroxide clusters, a structurally and compositionally diverse class of basic Bi3+ complexes formed during hydrolysis of the solvated Bi3+ ion, remains elusive and as a result underutilized. Our observations suggest that these Bi3+ cluster compounds show great potential for environmental remediation applications, due to their flexible structural arrangement and ability to sequester electronically and sterically different anionic species including chromate, pertechnetate, iodate, and uranyl, among other ground water contaminants. The related results including structural characterization and sorption behavior of the Bi3+ cluster compounds will be presented.

Abstract ID: 673

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: Dielectric Elastomer actuator, Biomimetic control, Wearable soft devices

Electrically active and controllable soft artificial muscle for smart wearable equipment

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Dielectric elastomer actuators (DEAs) are now popularly referred to as one of the promising artificial muscle in the field of soft devices. Though various types of DEAs have been reported, there are still some challenges such as low-actuating force, unpredictable force-displacement relationship and single driving mod. Inspired by natural muscle fibers, this paper proposed a cone-like DEA in series with replaceable stacked multiple layers structure. With each cone-like DEA there are three annular actuating region which provide different actuating mods. The actuator could increase the actuating force by connecting multiple cone-like DEA and it provided a linear force-displacement relationship in fixed displacement test. And we also built a biomimetic control strategy for a four-DEAs system. Combination of multiple actuating mods provided a possible way to create a actuating mod similar to that of natural muscles. Due to the actuating characters of cone-like DEA, it's safer to grab a tough project. This paper also proposed a smart-controlled assisted rehabilitation kneecap with plate stacked DEA. The kneecap controlled by nonlinear model-based feedback system recognize the motion of body and provide the suitable tension force to protect the cruciate ligament in severe exercise. These applications may provide a new idea for the design of the DEAs.

Abstract ID: 674

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Manufacturing and formation techniques

Keywords: Material amorfo, PET, Thermal Cristallization

Thermal Crystallization of Polyethylene-Terephthalate, as a Contribution to Sustainable Development

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Introduction

Mexico is one of the main consumers of PET worldwide. In Mexico, urban solid waste has not received adequate attention due to a series of factors of various kinds, among which are: Collection of mixed garbage (in 95% of the national territory) [1, 2], public services insufficient and inefficient cleanliness, poor coordination between the different levels of government, incomplete legal framework and legislative work with a particular vision, passivity in ecological matters and little culture of recycling in society [3, 4, 5], dependence on international prices of the residues that serve as raw material [4], which leads to seasonal stockpiling.

According to data reported by the Ministry of Social Development (SEDESOL, 2014), the generation of this type of waste throughout the country was 94,800 tons per day, equivalent to 34.6 million tons per year. The technology to recycle solid waste has evolved [3], but not the practices to create incentives to recover it in an economically viable way.

Sustainable development, as it is currently disseminated, begins in 1983, when the United Nations (UN) created the Commission on Environment and Development, chaired by Gro Harlem Brundtland, who was Prime Minister of Norway. The task force, also known as the Brundtland Commission, carried out studies, analyzes, and public consultations [6], all over the world, for approximately three years, ending in April 1987, with the publication and dissemination of the report called Our Better Common Future known as The Brundtland Report [7]. document that clearly states that society must modify its lifestyle and habits, if the social crisis and the degradation of nature are not to spread irreversibly [8]. The objective of this study was to determine the temperature at which polyethylene terephthalate (PET) in the form of granules, changes from amorphous to crystalline, since recrystallization improves the properties, which is necessary for the reuse of the material.

Abstract ID: 675

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Metamaterials and Materials for THz, Plasmonics and Polaritons

Keywords: Plasmonics, THz, highly mismatched alloys

Highly mismatched alloys as a new platform for mid-IR plasmonics

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Highly mismatched alloys (HMAs) are semiconductors with strongly modified band structures due to the alloying of elements with strongly different electronegativities. Their band structures have been well described using the band anticrossing (BAC) model,1 according to which the alloy interaction splits the conduction or valence bands. In the case of a conduction band (CB) anticrossing, the CB splits into an upper (E+) and lower (E-) band, with a rapid change in the band gap as the alloy concentration changes. This large tunability has been used in LEDs and multijunction solar cells. We present these materials as plasmonic resources. We describe the unique plasmonic properties of HMAs with conduction band anticrossings when the E- band is occupied, either by doping or photoexcitation- Using a disorder-averaged Green's function method, which goes beyond the BAC and approximately accounts for the alloy disorder, we determine the bulk plasmon frequency2 and the E- to E+ absorption spectrum. We show the distinctive signatures of the direct and indirect absorption processes, which are different from those in standard semiconductors. We further describe a nonstandard scaling of the plasmon frequency, which does not reduce to the free-electron-gas form even when doping is low and the band is well approximated as parabolic. The proven tunability of HMA band structures permits a wide variety of plasmon frequencies to be realized, with the most commonly considered HMAs having resonances in the mid-IR. This exploration helps open up this new material class for plasmonic development.

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Abstract ID: 676
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Nanocomposites
Keywords: Key Words: Epoxy, Nanoclay, relaxation modulus, interface

Epoxy Nanoclay composites

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Enhanced properties of nanocomposites are strongly dependent on particular features of the second-phase‘particles’; in particular, the particle volume fraction;The presence of nanoparticles introduces an enormous amount of interfacial area in which polymer chains undergo conformational changes and deformations at the nanoscale (1). Computational methods cover quantum mechanical scale, atomistic domain (Monte Carlo and molecular dynamics), mesoscopic scale (Brownian dynamics, dissipative particle dynamics, and lattice Boltzmann method), and finally macroscopic realm (finite element and volume methods). Nanocomposites have been modeled in a multiscale covering from molecular scale (e.g., molecular dynamics, Monte Carlo), microscale (e.g., Brownian dynamics, dissipative particle dynamics, lattice Boltzmann, time-dependent Ginzburg–Landau method, dynamic density functional theory method) to mesoscale and macroscale (e.g., micromechanics, equivalent-continuum and self-similar approaches, finite element method) Epoxy resin nanocomposites based on diglycidyl ether of bisphenol A (DGEBA) were studied using this approach Nano clays organically functionalized were mixed with Epoxy in a high shear mixer. Viscosity, normal stresses and dynamic viscoelastic measurements at various temperatures were determined. Elastic and viscoelastic modulus as function of frequency was used to get relaxation modulus by using transformation functions. Relaxation modulus as function of time at different temperatures was used to get power law fits. Relaxation modulus at different crosslinking level in the nanocomposite shows large difference from nanocomposite with uncrosslinked epoxy. These structures by X-ray diffraction and TEM showed significant exfoliation.

Key Words: Epoxy, Nanoclay, relaxation modulus, interface

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Abstract ID: 677
Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)
Poster Presentation
Topics: Correlated Electrons
Keywords: Correlated Electrons, Quantum Hall effect(s), Anisotropy

Two-dimensional finite quantum Hall clusters of electrons with anisotropic features

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Low-dimensional nano and two-dimensional materials are of great interest to many disciplines and may have a lot of applications in fields such as electronics, optoelectronics, and photonics. One can create quantum Hall phases by applying a strong magnetic field perpendicular to a two-dimensional electron system. One characterizes the nature of the system by looking at magneto-transport data. There have been a few quantum phases seen in past experiments on GaAs/AlGaAs heterostructures that manifest anisotropic magnetoresistance. In this work, we model the source of anisotropy as originating from an internal anisotropic interaction between electrons. We use this framework to study the behavior of finite clusters of electrons constrained in the lowest Landau level.

Abstract ID: 678

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Sensors and MEMS: Materials and Devices

Keywords: rice husk ash, eggshell, sol-gel, optical materials, photoluminescence

CaSiO3:Eu3+ red-emitting phosphor derived from recycling materials

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Eu3+- activated calcium silicate (CaSiO3:Eu3+) phosphor powders were prepared by modified sol-gel method in the absence of organic solvents. The main purpose of this manuscript was preparation of β-Wollastonite using rice husk ash (RHA) and eggshell (ES) were the starting materials for silica and CaO sources. Raw materials composition was analyzed with the help of X-ray fluorescence (XRF). As prepared phosphor powder samples structure properties were studied using TG/DTA, X-ray powder diffraction (XRD), Fourier transform infrared (FTIR). Optical data carried out by Uv-Vis (DRS), X- ray photo electron spectroscopy (XPS) and photoluminescence (PL). The XRD studies reveals the monoclinic structure with space group P21/C sintered at 800 °C. The CaSiO3:Eu3+phosphor shows peculiar emission at 612 nm due to 5D0→ 7F2 transition band. The CIE diagram shows the (x,y) co-ordinates (0.58,.035) which falls in the red region. These results suggest that the as prepared sample was the eco-friendly phosphor may be potential candidate for lighting applications

Abstract ID: 679

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Epitaxial Materials and Devices

Keywords: Room Temperature Multiferroic, Epitaxial Thin Films, Nanocomposite

The Quest for new Thin Films and Heterostructures Multiferroic at Room Temperature

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Multiferroic are a special class of smart materials that exhibit both ferroelectric and magnetic properties and have generated great interest for a variety of applications, ranging from spintronic devices to novel photovoltaic devices, and from cryogenic-free highly-sensitive magnetic sensors to innovative non-volatile memories. However, obtaining materials with ferroelectric and magnetics properties that are sufficiently strong and robust at or above room temperature for potential integration into novel devices remain elusive. The search for thin films and heterostructures of new materials with good multiferroic properties at room temperature remains a major challenge, especially since the existence of good ferroelectric and magnetic properties does not guarantee the existence of a strong coupling between them.

Consequently, several strategies have been pursued in the quest for thin films and heterostructures of novel multiferroic materials with good multiferroic properties at room temperature. Some of these strategies will be presented, exemplified by different thin layers and heterostructures that have been synthesized and that are multiferroic at room temperature. The characterization of the structural and functional properties of these room temperatures multiferroic thin film systems, including at the ultralocal scale, will then be presented and discussed in detail. Finally, some perspectives on this fascinating class of materials and their potential applications will be presented.

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Abstract ID: 680
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Bio-inspired design of composites
Keywords: Silk, LLPS, Cryo-EM, NMR, IR imaging

Informing Tunable Bio-composite Design with Fiber Formation in Spiders and Silkworms

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From graphene oxide to polyvinyl alcohol, silk fibroin has been combined with a variety of materials to form composites suitable for a wide range of biological applications. Biocompatible and biodegradable, silk is also extremely versatile – a single spider produces seven different types of silk, each with unique properties such as exceptional strength or extensibility. Creating equally versatile silk composites is of great interest; while micron-sized fibers are an ideal scaffold for nerve repair and regeneration, flexible films provide the perfect foundation for bio-integrated electronic devices. However, though silkworm silk is readily available, industrial scale synthesis of composites using spider silks is not currently feasible as spiders are cannibalistic and cannot be housed in large quantities. Furthermore, current attempts to produce synthetic fibers have resulted in a material that is inferior to native silk, which boasts the strength of steel and the toughness of Kevlar®. To successfully reproduce this resourceful material and tune its mechanical properties to suit an assortment of bio-composite applications, we must first understand the native silk spinning process.

Though the properties of spider and silkworm fibers have been thoroughly analyzed, there is still a gap in our understanding of how the starting material, a protein-rich hydrogel, develops as it travels down the duct of the silk gland, where it is exposed to shear forces, an acidic pH gradient, and increasing phosphate concentration. In this study, the structural changes in silk protein hydrogels from both spiders and silkworms are analyzed at the atomic, molecular, and mesoscales using a combination of cryo-electron microscopy (cryoEM), Nuclear Magnetic Resonance (NMR) spectroscopy, and Infrared (IR) imaging while mimicking the changing environment within the duct. Replicating the bottom-up, hierarchical assembly of native silk fibers within the duct and understanding how this process affects the mechanical properties of fibers are necessary for developing tunable, synthetic silks that can be integrated into the production of bio-composite materials.

Abstract ID: 681

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Solar Cells

Keywords: Halide Perovskites, Machine Learning, Nanoscale Imaging

Probing Stability in Halide Perovskites Solar Cells from the Macro to the Nanoscale

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A comprehensive understanding of the effect of the individual and combined effects of extrinsic (humidity and oxygen) and intrinsic (light, bias, and temperature) stressors on halide perovskites is crucial for the ultimate development of stable optoelectronic devices. Here, we present a suite of optical and electrical complementary tools that provide a detailed description of the dynamic responses within these materials. We unfold the impact of distinct humidity levels on charge carrier radiative recombination in CsxFA1−xPb(IyBr1−y)3 perovskites through in situ PL, where we temporally and spectrally measure light emission within loops of critical relative humidity (rH) levels. Our results demonstrate that the Cs/Br ratio strongly affects the spectral stability of light emission hysteresis, as well as its extent [1]. The photo-emission dynamics in metal halide perovskites with both I and Br is also interrogated by environmental PL, where we find that the presence of Br suppresses hysteresis. We realize a machine learning (ML) approach based on supervised learning combined with environmental PL measurements and determine the (ir)reversible changes that takes place in MAPbBr3 and MAPbI3 model systems, and in state-of-the-art multication compositions such as Cs0.05FA0.79MA0.16Pb(I0.83Br0.17)3 and (Cs0.07Rb0.03FA0.76MA0.14Pb(I0.85Br0.15)3 [2]. We further resolve transient processes such as ion motion by spatially resolving the local photovoltage and photocurrent at the nanoscale [3,4]. Here, we quantify how the addition of Rb reduces the inactivity of the perovskites' grains. Combined, the macro- and nanoscale environmental measurements performed provide a comprehensive platform for tracking, in real-time, the relevant changes that can lead to degradation. Moreover, they represent a reliable diagnosis tool that can be expanded to any perovskite chemical composition.

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Abstract ID: 682

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Synthesis and characterization of Composite materials

Keywords: transition metal oxides, elemental analysis, oxygen vacancies

A Correlation Between Oxygen Vacancies and Elemental Analysis in Single and Binary Transition Metal Oxide Structures

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Metal oxide structures are so important to develop opto-electronic devices, catalysis systems, gas/bio sensors, solar cells and etc [1]. However, chemical growth process of metal oxides is so complicated with un-control growth rate and increasing agglomerative forms on the surface [2]. In the literature, elemetal ratio (w%) is generally used to determine elements on the structure (film or nanoparticle) surface.

In this study, single (ZnO, TiO2, SnO2) and binary components were investigated to determine oxygen vacancies using simple elemental analysis results supported by XRD, SEM and PLmeasurements. With increasing oxygen elemental ratio up to 50 % and low metal elemental ratio have an impact on the agglomerative forms due to un-homogeneous solution and increasing metal(OH)2 forms [3]. Our aim in this study, local point defects especially oxygen vacancies can correlate agglomerative forms therefore high oxygen elemental ratio.

Abstract ID: 683

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Electrode/electrolyte interface phenomena
Keywords: solid–electrolyte interphase (SEI), alkali metal plating, liquid phase TEM, electrochemical liquid cells, Na deposition

In-situ Study of Electrode Electrolyte Interface Phenomena Using Liquid Cell Electron Microscopy

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We study alkali metal (e.g., Li and Na) plating and stripping in situ using liquid cell transmission electron microscopy (TEM)1-3. As a passivation interfacial film formed from the reduction of the electrolyte, solid–electrolyte interphase (SEI) plays an important role in the cycle stability of Li-ion batteries. Many efforts have been devoted to an understanding of the nature of SEI through various microscopy and spectroscopic approaches, including in situ x-ray scattering, and neutron reflectometry. In situ observations are beneficial as it avoids complications due to sample exposure to air and moisture. In situ liquid cell TEM imaging with nanoscale chemical analysis complements these studies. Liquid phase TEM observations and nanobeam diffraction of SEI on the electrode revealed that the SEI layer contained LiF nanocrystals distributed in an amorphous matrix,1 in contract to the previous understanding of a denser layer of inorganic components adhering to the electrode with a porous organic outer layer exposing to electrolyte. Further advances of electrochemical liquid cell TEM allowed the mapping of spatially resolved SEI chemistry on individual lithium nanograins.2 The observation revealed that Li dendrites can be suppressed by a cationic polymer coating on the electrode, thus uncovering a potential path to Li dendrite suppression.

Abstract ID: 684

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Sensors and MEMS: Materials and Devices

Keywords: Implantable sensors; oxygen sensors; pH sensors;, ischemia; hypoxia; electrochemistry;surgery

Micro-Implantable sensors for tissue ischemia monitoring: In vivo prevalidation

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Hypoxia is a common medical problem, sometimes difficult to detect and present by different situations such as intrauterine growth restriction, anastomosis failure in free flaps reparative surgery, compartmental syndrome, among others. Control of hypoxia is of great medical importance and early detection is essential to prevent life threatening. The lack in current commercial technologies of an easy and affordable method for early detection of ischemia makes the gold standard procedure for such monitoring based on frequent clinical observation. However, on deep/buried flaps, clinical observation cannot be done, and blood perfusion complications are detected too late, when the free flap salvage rate is very low and its required new tissue extraction.

Our developed technology is an ideal candidate for this unmet need. We have developed a micrometric array of sensors for the minimally invasive control of post-operative tissue ischemia. The implantable sensor for ischemia monitoring in tissue was closely development with a medical team and optimized in vitro and pre-validated in vivo in blood and intramuscular tissue in adult rabbits' model and sheep foetus model. The hypoxia was induced by restriction of the breathing oxygen in the adult animal and umbilical cord occlusion in the foetus showing successful response [1, 2, 3]

Abstract ID: 685

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Nanoparticles, Nanowires, and 3D Structures

Keywords: Copper nanoparticles, Electroless Plating, Conductive materials, SEM, LAser treatment

Development of the Textile Conductive Nonwoven by Copper metal coating approach for E-Textile Applications

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This Study presents manufacture and characterizes the polyester nonwoven fabric through the copper metal coating approach. Thus, we selected a polyester nonwoven fabric sample to see the effect of different properties on the conductivity of the samples.

I investigated the physical properties of polyester nonwoven samples such as thickness, the durability of the fabric, and the impact of abrasion on the normal and conductive samples. I also explored the surface morphology of polyester nonwoven sample before and after the coating process via scanning electron microscope (SEM) and it showed a remarkably uniform deposition of copper metal particles on the fabric surface and performed the energy dispersive spectroscopy (SEM-EDX) analysis to determine the elemental composition on the surface of the fabric after the metal coating process.

The results revealed that polyester nonwoven sample showed excellent conductivity value (3.3729e-2S/cm) and could be ideal for Electronic textile applications such as sensors

Abstract ID: 686

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Design and application of composite structures

Keywords: Cardiac disease, Troponin-T (Tpn-T) biomarker, Nanoscale zero-valent iron (NZVI), Gold nanoparticles (AuNPs), Impedimetric assays

Ultrasensitive electrochemical immunosensing of cardiac troponin-T biomarker based on gold nanoparticles coated nanoscale zero-valent irons

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Early, inexpensive, reliable and accurate diagnosis of cardiovascular abnormalities has become of crucial importance to prevent and halt their progression. Herein, we report a label-free electrochemical magnetoimmunosensing for monitoring cardiac diseases through qualitative and quantitative detection of cardiac troponin-T (Tpn-T) in aqueous solution. In this context, a nanocomposite of gold nanoparticles coated a magnetic nanoscale zero-valent iron core (NZVI©Au) is employed as a substrate to facilitate the electron transfer and to bind more primary Tpn-T antibodies. The immunosensing platform consists of an anti-cardiac troponin-T antibody (Tpn-T-ab) modified NZVI©Au magnetic membrane attached onto a boron doped diamond (BDD) electrode. Sensing experiments were performed by the imposition of an external magnetic field at the backside of the electrode. The sensor response was performed using impedimetric assays, wherein the increase in the electron transfer resistance (Rct) correlated with an increase in the concentration of Tpn-T. Linearity was obtained in the range from 1 fg/mL to 109 fg/mL with a detection limit of 0.354 fg/mL. The proposed platform exhibited high selectivity, high reproducibility and good stability, whilst retaining more than 90 % of the sensitivity after two weeks of storage at 4° C. The determination of Tpn-T is well compared with previously reported methods and has been successfully tested in serum samples. This encouraging result suggests that the developed sensing strategy provides a high potential for the early assessment of Tpn-T in point-of-care testing applications.

Abstract ID: 687

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Optical properties of metals and non-metals

Keywords: Metal-Organic Frameworks, Photoluminescence, Vapor Sorption Properties, Rhenium Complexes, Heterometallic Compounds

Solvato- and Thermochromic Photoluminescence in Hofmann-type Sr–Re Metal-Organic Frameworks

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The scientific interest devoted to photo- and electroluminescent materials is related to their applications in light-emitting devices, optical communication, sensing, and bioimaging. Particularly important are novel emissive solids showing the strong temperature dependence of luminescence that could be used for the new generation contactless optical thermometers. Aiming at smart devices that can realize multiple operations at once or exploit new physical cross-effects, the idea of multifunctional luminescent systems has recently emerged. We focused on the simultaneous generation of luminescent solvato- and thermochromic effects. The resulting multi-switchable luminophores can be employed in the construction of optical thermometers switched by solvent exchange whose operating temperature range may be tuned by chemical treatment. In this context, we combined [ReV(CN)4(N)]2– metalloligands, with strontium(2+) ions and N,N-bidentate organic spacers, 2-bis(4-pyridyl)ethane (bpen), 1,2-bis(4-pyridyl)ethylene (bpee), or 4,4-bipyridine (bpy). This results in a unique family of 3-D bimetallic coordination polymers showing green-to-orange photoluminescence related to the formation of {ReV–(bpen/bpee/bpy)–ReV} linkages. The Sr(bpy)–Re material exhibits three interconvertible phases, hydrated, MeOH-solvated, and desolvated, due to the water and MeOH sorption properties, which leads to the luminescent solvato- and thermochromism.

Abstract ID: 688

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanomaterials and Nanotechnology

Keywords: Boron nitride nanotubes, single-electron transistors, atomic chains, fluorescence spectroscopy, flow cytometry.

Emerging Applications of Boron Nitride Nanotubes for Advanced Electronics and Bio-imaging

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The electrically insulating and optically transparent boron nitride nanotubes (BNNTs) have found novel applications in advanced electronics and bio-imaging. Although these physical properties are not favorable for conventional electronics and energy applications, recent advancement in controlled synthesis of BNNTs has enabled the demonstration of a series of unique application. [1-3] For example, BNNTs are unique one-dimensional templates for room-temperature single-electron transistors (SETs) [4], two-dimensional gold quantum dots with tunable optical bandgap [5], field-effect transistors (FETs) by van der Waals atomic chains [6], and immunophenotyping by flow cytometry [7]. Details of all these emerging applications will be discussed in the meeting.

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Abstract ID: 689

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Single molecule, ion and chains magnets (SMM, SIM and SCM)

Keywords: Lanthanides, Single-Molecule Magnets, Luminescent Thermometers

Molecular d-f cyanido-bridged systems for the construction of magnetic luminescent thermometers

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Among modern magnetic materials, single-molecule magnets (SMMs) gather enormous scientific interest due to the perspective applications in high-density data storage and molecular spintronics. Last several years of research in this field indicated that achieving the best performance SMMs is ensured by the exploration of lanthanide(3+) ions. At the same time, 4f metal complexes were highly recognized for their emissive properties utilized for chemical sensors or light-emitting devices. Therefore, lanthanide-based molecular materials combining magnetic and photoluminescent features were also reported, enabling the correlation between single-molecule magnetism and the electronic structure illustrated by the emission spectra. Moreover, lanthanide luminescence can be efficiently exploited for the construction of luminescent thermometers whose emission signal serves for contactless temperature sensing. Lately, the idea of constructing optical thermometers using molecular nanomagnets emerged due to their prospective application for magneto-optic devices with self-monitored temperatures. We present two examples of such magneto-luminescent materials built of cyanido-bridged d-f molecules, including NIR-emissive {YbCo2} species and {HoM} (M = Co, Rh, Ir) molecules exploring a luminescence re-absorption effect.

Abstract ID: 690

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Computational Electronic Materials

Keywords: Micropore Materials

Ferromagnetism in 2D organic iron hemoglobin crystals based on nitrogenated conjugated microporous materials

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In this work we study an environmentally stable, low-cost two-dimensional ferromagnetic semiconductor with possible applications in biomedicine, solar cells, spintronics, and energy and hydrogen storage. From first principle calculations we describe the unique electronic, transport, optical, and magnetic properties of a pi-conjugated microporous polymer (CMP) with three iron atoms placed in the middle of an isolated pore locally resembling heme complexes. We then study the stability of this material to an environment and how these properties change when bonded with CO, CO2, and O2. This material exhibits strong Fe-localized dz2 bands with a direct bandgap of 0.28 eV. The absorption coefficient and conductivity are roughly isotropic with conductivity in the energy range 0.3 - 8 eV. The material shows nonzero Faraday and Kerr rotation in the interval of 0.5 - 5.0 eV. This material is found to be a ferromagnet of an Ising type with long-range exchange interactions with a very high magnetic moment per unit cell, m = 6 +B. The estimated exchange integral is calculated to be about Jnn= 25 meV. The binding of CO, CO2, and O2 modifies the dz2 bands of the Fe ions with varying profiles and results in indirect bandgaps with values between 0.269 - 0.626 eV, 0.039 - 0.434 eV, and 0.291 - 0.347 eV for CO, CO2, and O2, respectively. The absorption coefficient becomes slightly anisotropic while conductivity remains isotropic with the same active energy regions. Both the absorption coefficient and conductivity have large modifications to the xy-components. The material remains ferromagnetic with the magnetic moment per unit cell decreasing to 4, 2, and 0 mu-B for gases attached to one, two, and three Fe ions per unit cell, respectively.

Abstract ID: 691
Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)
Invited Talk
Topics: Functional Magnetic Materials
Keywords: Molecular Nanomagnets, Luminescence, Multifunctionality, Hybrid Materials, Coordination Polymers, Rare-Earth Metals, Cyanides

Luminescent Multifunctional Magnetic Materials based on Hybrid Rare-Earth Hexacyanidometallate Frameworks

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Diverse physical functionalities, including magnetic, optical, dielectric, and mechanical, can be incorporated in hybrid organic-inorganic molecule-based materials composed of bimetallic cyanido-bridged coordination frameworks.1 Among them, considerable interest has been recently devoted to the rare-earth hexacyanidometallate frameworks which appear to be promising candidates for the construction of luminescent molecular nanomagnets showing the broad application perspectives in high-density data storage and processing, molecular spintronics, quantum computation, switchable light-emitting devices, and chemical sensors.2 They explore the great potential in the tuning of magnetic anisotropy and sensitized photo-luminescence of rare-earth metal ions, mainly lanthanide(III) complexes.3 In this regard, we present our recent achievements in the synthesis of luminescent multifunctional magnetic materials taking advantage of the fruitful combination of magneto-luminescent lanthanide(III) complexes with hexacyanidometallate anions of transition metals, such as Co(III), Rh(III), and Ir(III). In particular, we present the dehydration-hydration switching effect on the luminescent molecular nanomagnets formed within the 3-D Dy^{III}–$[Co^{III}(CN)_6]^{3-}$ coordination framework,4 and the rationally designed multifunctional material of a proton-conductive luminescent thermometer based on Yb(III) complexes bonded to Co(III) cyanido complexes.5 We discuss the essential role of the thoroughly selected rare earth metal complexes and the non-innocent contribution given by the attached cyanido-based metalloligands.

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Abstract ID: 692
Symposium 4: Functional Composite Materials (FCM)
Poster/Oral Presentation
Topics: Bio-composites
Keywords: Gold Nanorods, Theragnostics, Nanocomposites, Photothermia

Cell Membrane-Covered Hybrid Nanocomposites for Target Photothermal Cancer Therapy

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The so-called theragnostic materials represent the state-of-the-art in the use of nanocomposites for targeting cancer diagnosis and treatment. Graphene oxides and gold nanorods (AuNRs), in particular, have been extensively applied as theragnostic agents for target cancer therapy due to their ability to absorb light in the near infrared region - where radiation penetration through tissues occurs-, which makes them appropriate for in vivo photothermal applications. In this paper we show the development of AuNRs covered with lung adenocarcinoma cell (A549) membranes, used for targeting and photohyperthermia essays in vitro and in vivo. The nanoconjugates presented higher toxicity to cancer cells compared to healthy cells used as controls. Additionally, significant differences were observed on how the AuNRs interact with the cancer and normal cells, as revealed by kinetics absorption and surface pressure measurements in Langmuir experiments. Our results show the potential of cell membrane-coated nanomaterials and open opportunities for the development of more efficient nanosystems for cancer applications.

Abstract ID: 693

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Polymeric composites

Keywords: Thermoplastic composite, micro-nano effect, PEEK, friction, wear

Microstructure evolution of silicon carbide reinforced PEEK under tribological solicitations

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Minimizing the environmental impact of human activities is a challenge going towards sustainable and efficient materials. New polymer matrix composite materials are elaborated for high-performance applications such as aerospace and aeronautics. We have developed innovating multifunctional composites with a polyetheretherketone (PEEK) matrix and silicon carbide (SiC) particles. Specimens are prepared with microparticles, or nanoparticles by melt-blending then shape by thermo-pressing.

While bringing higher mechanical strength, this process improved the tribological performances of our semicrystalline thermoplastic material.

Our research focused on microstructure changes under tribological strain in the PEEK matrix, and the effect of silicon carbide particles on this tribological behavior.

We have performed sliding tests with ball-on-plate configuration and reciprocating translation motion. The plastic deformation dominates the accommodation mechanisms, and the material loss is reduced with SiC addition. Moreover, our results highlight the microstructure changes of PEEK and the composites due to the tribological solicitations: with Raman spectroscopy, we have followed locally the crystallinity rate evolution in the wear track and depending on tribological tests duration. We conclude that the crystallinity rate decreases with the contact pressure and the tribological test timespan.

Abstract ID: 694
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Recycling and sustainability of composite materials
Keywords: Inner Tubes, Gamma Rays, Properties

STUDY OF MECHANICAL AND CHEMICAL PROPERTIES STABILITY OF INNER TUBES EXPOSED TO GAMMA RADIATION

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Nowadays, car tires are not provided with inner air or tubeless, pointing toward a technical evolution. Nevertheless, trucks tires even use at present inner tires, composed almost fully by a synthetic material, which ensures either a good potential for air constraint or longer periods for inspection of tires pressure. Inner tire is located inside the tire which does not have any extra sealing in the wheel to withstand compressed air. It is designed to resist to expansion of these elements, inside common tir es. This rubbery and vulcanized coating has chemical and physical characteristics which enable it to bear a very high air pressurization, avoiding leakages while protects tire outer frame. Inner tires models are exposed to higher temperatures and pressures that contribute to accelerate abrasion. This work aims to the study of mechanical properties changes of an inner tire used in trucks, after gamma rays exposure, in order to promote further material recycling. Ionizing radiation choice was due to its capacity to modify materials structure and properties besides its applicability for rubbers recycling/recovery. For samples characterization, non-irradiated and irradiated at 5, 10, 15, 20, 25 and 30 kGy, there were accomplished following tests: tensile and elongation at break, hardness, thermal ageing and CHN elementary analysis. It was observed a decrease in mechanical properties for irradiated samples at doses higher than 20 kGy

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Abstract ID: 695

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanoparticles, Nanowires, and 3D Structures

Keywords: Nanowires, Vapor-liquid-solid growth, Impurity doping

Calculation of hole concentrations in Zn doped GaAs nanowires

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III-V semiconductor nanowires have proven to be excellent nanoscale light emitters with several important applications, most prominently in light emitting diodes. In order to fabricate such pn-junction based devices we need to control the conductivity. For this reason we need to be able to p- and n-dope the nanowires but also understand the doping mechanisms. Here, thermodynamic knowledge of the nanowire-catalyst particle materials system is key.

We have previously demonstrated that we can grow p-type doped GaAs nanowires using aerotaxy [1]. This is a method where the nanowires are formed in the gas phase without substrate [2]. It is a continuous process, where a large amount of nanowires per time unit can be produced. Thus, it is very promising for upscaling and for industrial production of nanowires. Moreover, the aerotaxy process also admits doping, which is necessary for electronic device fabrication.

In this regard we have experimentally controlled the hole concentration by varying the Zn/Ga ratio during aerotaxy growth.

In this investigation we demonstrate that we can calculate the hole concentration in Zn-doped, gold alloy catalyzed GaAs nanowires grown by the VLS (vapor-liquid-solid) mechanism. We base the calculation on the defect formation energy proposed by Zhang and Northrup [3]. Using density functional theory (DFT), we calculate the energy of the defect, a Zn atom on a Ga site, using a supercell approach. The chemical potentials of Zn and Ga in the liquid catalyst particle are calculated from a thermodynamically assessed CALPHAD (CALculation of PHAse Diagrams) database including Au, Zn, Ga, and As. Using these quantities together with the chemical potential of the carriers, we calculate the hole concentration self-consistently.

Our calculations compare well with the experimental hole concentrations in the Zn-doped GaAs nanowires grown by aerotaxy. Specifically, it is interesting to note that the calculations confirm our experimental observation that it is difficult to achieve low and intermediate doping levels. Except for very low Zn concentrations in the catalyst particle and low growth temperatures, the hole concentration in the nanowire tends to be high (around 1019 cm-3 and higher).

To conclude, we demonstrate reasonably accurate calculations of the doping concentration of VLS grown nanowires using a combination of DFT and CALPHAD. Such calculations are of great advantage when controlling and predicting the doping concentrations for a wide variety of experimental conditions.

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Abstract ID: 696

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Sensors and MEMS: Materials and Devices

Keywords: Sensor, Semiconductor, Photo-activated material

Photoactivated Functionalized Semiconductors as Sensing Devices

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The advent of the wireless sensor network, a group of spatially dispersed and dedicated sensors, could ultimately result in a more comprehensive understanding of global environmental patterns and even lead to addressing certain challenges related to climate change. Deployment of a global-scale sensor network would introduce unprecedented benefits but it would also present new challenges, one being the development of next-generation highly sensitive, selective, and low-cost sensor technologies. Limitations with current chemical sensors are that they operate at high temperatures (200°C to 500°C), resulting in major challenges with lifetime, stability, energy efficiency, and usefulness in environments with potentially explosive gas components. The use of functionalized photoactivated semiconductors activated by UV-LED irradiation serves as an attractive alternative method for sensing materials, which could lead to fabricating highly effective sensors that operate at ambient temperatures.

To fabricate highly effective photo-activation sensors that operate at ambient temperature, we synthesized metal-oxide sensing materials, where the electrochemical properties of the semiconductor were significantly enhanced by integration with metal nanoparticle composites. This combination resulted in lowering the required activation energy and reducing the recombination rates of the photo-generated charge carries. This in turn led to significant enhancement in the sensor sensitivity (over an order of magnitude) and shortening the response time. Overall, the incorporation of nanoparticles showed great potential for the detection of toxic gases at very low concentrations.

We will present the fabrication of a sensitive nanostructure ZnO gas sensor decorated with Pt nanoparticles [1] and doped with Ag nanoparticles [2]. Further, we will demonstrate our latest results on the application of the sensors for the detection of low concentrations of toxic gases such as NO2 under UV-LED irradiation. We will discuss how functionalized photoactivated semiconductors have the potential to significantly impact sensor development and portable gas monitoring systems by enabling novel sensor design concepts.

Abstract ID: 697

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Dielectric, Ferroelectric and Piezoelectric materials

Keywords: Ferroelectronics, Ferroelectric-nanocrack, Zero off-current, Logic-in-memory

Ferroelectric Nanocrack-based Nanoelectromechanical Switches for Memory and Complementary Logic

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The power consumption is one of the most challenging bottlenecks for electronic devices. Nanoelectromechanical (NEM) switches offer a promising platform to break the Boltzmann Tyranny and thus enable to construct energy-efficient electronic devices. NEM switch enables near-zero leakage current and steep subthreshold slope relying on the electrostatic force to form or remove an air gap between source and drain, but usually has a much complex structure [1,2]. Therefore, We constructed a NEM switch with a controllable ferroelectric-nanocrack employed (001)-Pb(Mg1/3Nb2/3)0.7Ti0.3O3 (PMN-PT) substrate/Mn50Pt50 heterostructure, which offers a simple and efficient way to manipulate the device resistance states with a high on/off ratio [3]. Meantime, ferroelectric devices utilize the polarization switching through voltage-control, offering great advantages in non-volatility, scalability and energy-efficiency. Such devices we proposed combine the advantages of nanoelectromechanical (NEM) switch and ferroelectricity. Further, the complementary switching of nanocracks has also been revealed and investigated, which operates like the CMOS technology [4,5]. Based on the ferroelectric-nanocrack NEM switch, we condense the memory and logic functions into a single device. Superior electrical performances in both on and off states have been demonstrated with metallic contacts at on state and zero off-state leakage current. Importantly, we focus on the scaling performance that is crucial for actual applications and find that the operating voltage can be largely reduced to average 2.5 V with device scaling down to sub-micrometers (300 nm node). Moreover, we predict sub-1 volt can be acquired at 100 nm nodes. In addition, a variety of logic gates including NOT, 2:1 MUX, AND and OR functions have been experimentally demonstrated in a single device, leading to less chip area consumption compared to the conventional CMOS technology.

Abstract ID: 698

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: All solid-state batteries

Keywords: STEM, EELS, solid electrolyte, dendrite

Beyond structural and chemical imaging in a TEM -- new opportunities for understanding interfaces in energy materials

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Electron microscopy has enabled imaging and chemical analysis of materials at the single atom level. Substantial contributions to energy materials research have been made in the past decade, especially to the investigation of interfaces, which often act as the bottleneck in next generation energy systems. Many critical interfacial questions remain open and answering them requires us to go beyond the conventional atomic-scale structural and chemical analyses. We must understand the behavior of the electrons and their dynamic evolutions under operation conditions. Recent developments in scanning transmission electron microscopy (STEM), including atomic-scale in situ imaging, four-dimensional (4D)-STEM, and monochromated electron energy loss spectroscopy (EELS) have opened up unprecedented opportunities. In this presentation, I will introduce these capabilities and highlight examples demonstrating how these capabilities allow us to reveal the origin of high interfacial resistance and of the unexpected dendrite growth in all-solid-state batteries, and directly observe anionic electrons in electrides for the first time. Perspectives for the future advancement of these new STEM techniques for research into emerging energy materials will also be provided.

Abstract ID: 699

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Quantum Dots, Blinking, Chalcogenides, Perovskites, Hot Electron, Halide Vacancy

Blinking Suppression of Chalcogenide Quantum Dots and Perovskite Quantum dots: Similarities and Challenges

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Blinking Suppression of Chalcogenide Quantum Dots and Perovskite Quantum dots: Similarities and Challenges

The size- and composition-dependent tunable emission color of cadmium chalcogenide quantum dots and lead halide perovskite nanocrystals is one of the most fascinating inventions in nanoscience and nanotechnology. These unique properties not only accompany these tiny crystals to various disciplines of basic research but also are promising for the development of brilliantly luminescent displays and high-efficiency photovoltaics. However, the photoluminescence and electroluminescence of these tiny crystals show stochastic fluctuations of intensity, also called intermittency or blinking on a wide time scale – from microseconds to minutes. Such blinking processes prevent the applications of these materials to on-demand light sources or quantum computing. Although the relations of blinking to the intensity and energy of incident photons as well as the nature and density of defects are widely investigated, the development of nonblinking quantum dots and nanocrystals is challenging. This presentation highlights the characteristics of photoluminescence blinking in cadmium selenide and lead halide perovskite quantum dots. Also, a correlation between ON and OFF times in photoluminescence and electroluminescence blinking of lead halide perovskite single particles will be presented, which will be in addition to blinking suppression by defect passivation or electron donation. The blinking time varies with the size, ligands, surface morphology, and composition of these tiny crystals. Other factors affecting photoluminescence blinking are the nature and density of defects, intensity and energy of incident light, and the degeneracy of band-edge states. When excited with high intensity or high-energy laser beam, blinking occurs mainly due to random charging and discharging, which is classified into type-A blinking. Another source of blinking is the activation and deactivation of traps or vacancies, which is called type-B blinking. The characteristics of photoluminescence and electroluminescence blinking are discussed by referring to type-A and type-B mechanisms as functions of the intensity of excitation light, the density of intrinsic defects, and the presence of electron donor/acceptor molecules.

Abstract ID: 700

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Photocatalytic and electrochemical water splitting
Keywords: Hydrogen production, Electrodeposition, Ir and Pt layers, Max Phases, acid solution

Ultra-thin Electrodeposited Noble Metals Layers on Max Phases Based Support for Green Energy Production

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Ultra-thin Electrodeposited Noble Metals Layers on Max Phases Based Support for Green Energy Production

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Hydrogen is considered as pure, high conversion efficiency fuel for prospective application in environmental friendly power sources. Pure hydrogen could be produced by water electrolysis. However, the main problem for hydrogen fuel production is still high energy consumption (~5 kW m-3 of H2). Thus, development of high efficiency catalysts for water electrolysis is still remained. We have established simple electrochemical method for deposition of thin layers of noble metals – Iridium and Platinum on Ti2AlC and Nb2AlC supports, respectively [1]. Namely, only several nanometers thick layers of noble metals were deposited and investigated as the cathode catalysts for hydrogen production in acid solutions. The synthesized catalysts exhibited high performance especially at industrial electrolysis working conditions, e.g. at high current densities (-0.3 A cm-2). Having in mind extremely high chemical stability, high conductivity and low cost production of Max phases based supports these novel catalysts could be considered as promising for efficient green energy production.

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Key Words: Keywords: Hydrogen production, Electrodeposition, Ir and Pt layers, Max Phases, acid solution

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Abstract ID: 701

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Novel Magnetic Materials and Device Applications

Keywords: magnetoelectricity, permittivity, viscosity, Maxwell-Wagner model

On a Novel Magnetoelectric Oxide Cu4O3

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A laboratory preparation of paramelaconite (Cu4O3), a member of the group of natural minerals even more rare than diamond, is anything but a straightforward task[1]. In this work, a Cu4O3 phase stable up to, at least, 923 K was prepared via reduction of a cupric-copper oxide CuO. XRD and magnetic data agree well with those reported on the mineral sample[2] , while magnetic susceptibility reveals an antiferromgnetic transition at 44,7 K. In contrast to other magnetoelectric materials, Cu4O3 exhibits a comparatively high electric conductivity 'sigma' = 110 S at room temperature (RT), most likely on behalf of the mixed valence structure Cu2+Cu22+O3.Electric conductivity was shown to depend on frequency, and yields a strong resonance feature at 46,4 kHz at RT. From electric conductivity and time relaxation measurements one can calculate a magnetic permittivity μr = 2370 and dielectric permittivity 'epsilon'r =6,6·10^6. Calculation of electronic densities of states (DOS) provides the route to the Jahn-Teller (JT) distortion, as a precondition for the stress exerted onto the crystal lattice. Similar to other strong dielectric materials, a solely microscopic approach to the problem does not explain the huge dielectric permittivity. Here, we employ a Maxwell-Wagner (MW) model which is based on the mesoscopic properties and put forward an effect referred to the literature as internal grain boundary barrier layer capacitance (IBLC).In this work the IBLC model was supplemented by a viscoelastic contribution on the grain boundaries, and use of the Maxwell-Voigt (MV) dashpot relaxation technique results in a Stieltjes-Riemann (SR) relaxation integral, while an application of the Lebesgue integration to SR gives back an extended form of the MW equation.

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Abstract ID: 702

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Computational modeling and simulation for energy storage and conversion devices
Keywords: Ortho-planar springs, Hybrid, Energy harvester, Low frequency

A compact low frequency ortho-planar spring based hybrid energy harvester

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The design of energy harvesters operating in a low-frequency range is still a critical issue: some solutions can be traced in the literature, either involving piezoelectric or electromagnetic transduction [1-3].

Starting from [3-4], this work proposes and investigates a simple and compact low-frequency hybrid energy harvester based on a couple of tri-legs ortho-planar springs [4]. The ortho-planar springs support a magnet which, under dynamic excitation, oscillates across the coils, thus providing electromagnetic conversion. In addition, piezoelectric transducers applied to the ortho-planar springs provide piezoelectric conversion.

Specifically, the converter has a cylindrical structure, about 60 mm in diameter and a height of about 40 mm: the ortho-planar springs on top and bottom enclose the magnet and the coils, these last ones constrained to the frame. Thanks to the peculiar architecture of the ortho-planar springs, the magnet has a large and perfectly axial stroke in both directions inside the coils.

The simple mathematical model in [4] allowed to dimension the ortho-planar springs to obtain a compliant system with an eigenfrequency below 10 Hz. An electromagnetic finite element model allowed to define the dimensions of the electromagnetic converter both regarding the number, diameter, and height of the coils and the magnet dimensions. DuraAct piezoelectric patch transducers [5] were applied to the springs.

The springs and the frame were manufactured through 3D printing, with carbon fiber reinforced Onyx material, using a Markforged Mark Two printer [6]. The layout of the carbon fibers was defined according to the desired stiffness of the springs.

A prototype of the harvester was manufactured and assembled, involving 500 coils, and two neodymium-iron-boron disc magnets (20 mm in diameter and 5 mm height). A DuraAct transducer (13 mm x 16 mm) was bonded to each of the three legs of the ortho-planar springs.

The preliminary experimental tests confirmed a fundamental frequency below 10 Hz with a good power output from both types of transducers.

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Abstract ID: 703
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Multifunctional composites
Keywords: iron oxide nanoparticles, diagnosis, treatment, thrombosis, inflammatory disease

Nanomaterials based on iron oxide for the diagnosis and treatment of cardiovascular and inflammatory diseases

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The most common form of cardiovascular disease (CVD) and also the leading cause of sudden death is atherosclerosis, a chronic progressive inflammatory disease of the arterial vessels. Unstable, vulnerable atherosclerotic plaques can rupture and cause thrombosis, resulting in myocardial infarction (MI) and stroke. Magnetic resonance imaging (MRI) has been used as a powerful and indispensable tool in medical research and clinical diagnosis due to its high spatial resolution and non-limited penetration depth. We have developed both targeted negative contrast agents and targeted dual positive/negative contrast agents for molecular imaging of atherothrombosis1,2,3. The simultaneous use of positive and negative MRI imaging that employs the same contrast agents will significantly improve the detection accuracy. Using these dual contrast agent, both T1- and T2-weighted MRI of thrombosis can be recorded simultaneously which enables self-confirmation of images and leads to a greater diagnostic accuracy. We have also designed and developed smart MRI nano-sensors that can not only detect, but also sense and report the stage or progression of CVD such as thrombosis4. The early detection and accurate characterization of life-threatening diseases such as CVD and cancer are critical to the design of treatment. Knowing whether a thrombus in a blood vessel is new/fresh or old/constituted is very important for physicians to decide a treatment protocol. Theranostic nanoparticles based on iron oxide and cerium oxide have also been developed in our group as potential materials for diagnosis and treatment of reactive oxygen species related inflammatory diseases such as CVD5. Another class of theranostic nanoparticles based on iron oxide and silver/gold with NIR absorption has also been synthesised as a potential material for the simultaneous detection and treatment of thrombosis.

Abstract ID: 704

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Nanocomposites

Keywords: 3D Printing, Halloysites, Polyurethanes, Shape Memory Effect

Shape-Memory Behavior of 3D-Printed Halloysite Nanotube Filled Thermoplastic Polyurethane Nanocomposites

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Additive manufacturing of smart polymers is an emerging field of research because the structure of these materials respond to external stimulus. 3D printing has been employed to print polymers with shape memory properties using Fused Filament Fabrication (FFF) machines. FFF machines are usually fed with expensive and commercially available filament feedstock. In this study, Plastic Freeforming (PF) has been employed as an alternative to common Fused Filament Fabrication (FFF). Plastic freeformer is fed with readily available standard polymer granulates as used for injection moulding. In this study, standard test specimens made of halloysite Nanotube (HNT) filled thermoplastic polyurethane (TPU) were processed by varying printing parameters to evaluate their impacts on the shape memory behavior of TPUs and its nanocomposites. Processing parameter such as such as infill percentage and raster angle on thermos-mechanical and shape memory behavior have been carried out. The obtained results indicated that, increase of infill percentage tend to increase the elastic modulus and tensile strength significantly and the decrease of print angle increased the elastic modulus. However, increasing the infill percentage decreased the significant impact of change of print angle on elastic modulus. The obtained results showed increase in maximum strain values as the infill percentage is increased except when the sample is printed at 0°. Further, highest infill percentage and lowest printing angle tend to increase the shape fixity and she recovery ratio. The results indicate that plastic freeforming is an effective technique for creating next generation 4D materials.

Abstract ID: 705

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Optical properties and spectroscopy of graphene and other two-dimensional materials

Keywords: MXene, Ultrafast Lasers, Fibre Lasers, Saturable Absorption

Ultrafast Mid-infrared Fibre Lasers Based on 2D Nanomaterials

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We report on the development of wavelength-stabilized all-fibre ultrafast mid-infrared laser systems that utilize MXenes and platinum diselenide (PtSe2) as novel two-dimensional saturable absorber materials for passive mode-locking.

The linear laser cavity consists of a high reflective femtosecond laser inscribed chirped fibre Bragg grating that provides wavelength selective feedback which is essential for stable operation. The observed mode-locked pulse train from this erbium-doped fluoride fibre laser cavity has a 30 MHz repetition rate with an average power of 603 mW and a transform-limited pulse duration of around 10 ps. Our results highlight the feasibility of using novel two-dimensional nanomaterials such as MXene and PtSe2 as promising candidates for the realization of all-integrated ultrafast fibre laser systems for the technically important mid-infrared wavelength region.

Abstract ID: 706

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: MoS2, WS2, Optical Fibers, Transition Metal Dichalcogenides, Excitons, Photoluminescence, Guided Wave, CVD

Functionalization of Exposed-Core Fibers with CVD-Grown Monolayer Transition Metal Dichalcogenides: Photolumiescence and Nonlinearity

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Monolayer transition-metal dichalcogenides [1] (TMDs) are a new and highly interesting material for optics and photonics due to their rich photophysics, their strong interaction with light, and large optical nonlinearities [2]. However, their usage in photonic applications is limited by the sub-nanometer interaction length, imposed by their atomic thickness; the enhancement of which is essential for future applications. Possible use-cases are also hampered by the difficulties in transferring monolayer crystals onto photonic circuitry, such as waveguides or optical fibers.

Recently, we have demonstrated a novel type of scalable functionalization technique for exposed-cored optical fibers (ECF) [3], where MoS2 and WS2 crystals are directly grown on the fiber's core. The growth is based on a one-pot chemical vapour deposition CVD process and leads to high quality monolayers crystals being grown directly on the core of the ECFs and in physical contact with the evanescent field of the fiber's guided mode. We show that by adjusting the growing condition, the density of TMDs monolayers can be tuned.

The TMDs interact with the guided light by the evanescent field of the ECF's guided mode, leading to exciton formation, photoluminescence (PL) emission, and enhanced nonlinear interaction, which can be excited through and detected by light being guided in the ECF. The incident light was launched into one facet of the fiber and the PL or nonlinearity generated light was collected from the other face. We observe guided-wave exciton emission at 678 nm and 622 nm for MoS2 and WS2, as well as enhanced third harmonic generation. Other forms of enhanced nonlinear effects will be discussed in the presentation, as well. We expect that our work opens new perspectives for TMD-based active, guided wave photonic circuits.

Abstract ID: 707

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: Cooling, heating

Giant caloric effects near structural phase transitions

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Research on phase transitions in advanced functional materials is widespread and continues to grow. Scientific interest aside, they are attractive for a wide range of current and future technologies that include computation, medical instrumentation, and energy conversion and storage.

During this talk, I will present my work on ferromagnetic, ferroelectric and ferroelastic phase transitions that permit large entropy changes to be driven by changes in magnetic field, electric field or stress field. The resulting magnetocaloric, electrocaloric and mechanocaloric (barocaloric and elastocaloric) effects promise new cooling technologies that are energy efficient and environmentally friendly [1,2].

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Abstract ID: 708

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Solar Cells

Keywords: Organic semiconductors, indoor applications

Organic photovoltaic devices for next generation indoor applications

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Organic photovoltaic devices have attracted significant interest for outdoor energy harvesting, as they have unusual properties including easy tunability of optical and electrical properties, and can be fabricated by low-cost, mass production methods. However, the potential for organic photovoltaic devices for indoor application (i.e. harvesting indoor light for self-sustainable electronics, e.g. power sensors) is much less explored. While there were a few initial studies on this topic, the power conversion efficiency of organic photovoltaic devices under indoor lighting (fluorescence lamp or white LEDs) is still low at that time. In 2016, our team revised the potential of organic photovoltaic devices for indoor applications by using the more state-of-the-art materials (at that time), which demonstrated good efficiency under indoor lighting. By exploring the design rules for indoor light harvesting, in 2018, we demonstrated a record high power conversion efficiency at that time (28% under 1000 lux fluorescent lamp: significantly better than silicon). These two crucial findings have then been leading to very active and significant amount of research on organic photovoltaic devices for indoor applications in the research community. In this talk, I will present the findings (and the design rules, and the perspective), and we believe that organic photovoltaic devices for indoor applications have much more promising potential to be commercialized (compared to outdoor applications), and can have significant impact on powering the "Internet of Things" for smart home, office, supermarket, buildings, etc.

Abstract ID: 709
Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)
Invited Talk
Topics: Nanoparticles, Nanowires, and 3D Structures
Keywords: Superstructures, Chiral, Directed Assembly, Optical Manipulation, Optical Spectroscopy

Reconfigurable Superstructures: Directed Assembly and Applications

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With their on-demand tunability of properties via precisely controlled spatial arrangement of building blocks, reconfigurable superstructures are promising for targeted applications with the optimum performances. We have developed a series of techniques for directed assembly of colloidal nanoparticles into reconfigurable superstructures in both solutions and solids. For example, opto-thermoelectric assembly and printing can construct colloidal particles into superstructures by coordinating thermophoresis and interparticle (or particle-substrate) depletion bonding in the solution. Localized laser heating generates a temperature gradient field, where the thermal migration of ions creates a thermoelectric field to trap charged particles. The depletion of ion species at the gap between closely positioned particles (or particles and substrates) under optical heating provides strong interparticle (or particle-substrate) bonding to stabilize colloidal superstructures with precisely controlled configurations and interparticle distances. Optothermally-gated photon nudging technique can assemble particles on a solid substrate. The solid-phase optical control of particles is enabled by the synergy of optothermal modulation of particle-substrate interactions and the optical scattering force as the driving force. Operated on the solid surface without liquid media, the photon nudging can avoid the undesired Brownian motion to manipulate individual particles with high accuracy. The assembled structures can be actively re-assembled into new configurations. We further demonstrate applications of the superstructures in chiroptical spectroscopy, optical enantiodiscrimination of chiral molecules, and chiral sensing of biomarkers in diabetes. With the arbitrary configurations of building blocks of variable shapes, sizes and compositions, and the on-demand control of the properties via site-specific manipulation of individual building blocks, reconfigurable superstructures by directed assembly will find more applications.

Abstract ID: 710
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Bio-composites
Keywords: Polymers, Glyconanoparticles, Nanostructured Materials, Biosensors, Biofuel Cells

Composite biomaterials based on polymers, carbon nanotubes glyconanoparticles and enzymes for energy conversion or sensor design

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For four decades, the functionalization of electrodes by biomaterials based on electrogenerated polymers, carbon nanotubes and / or nano-objects, was widely used in the field of analytical chemistry and energy conversion for the design of biosensors and biofuel cells. Some new approaches for developing nanostructured biomaterials based on functionalized carbon or tungsten nanotubes, glyconanoparticles and compressions of carbon nanotubes will be illustrated with enzymes or antibodies as catalytic or biosensing element [1-3].

In particular, the anchoring of biological macromolecules to the surface of electrodes has been carried out by chemically functionalizable electrogenated polymers. In addition, the self-assembly of carbon nanotubes via crosslinking polymers in the form of buckypapers was used for the grafting and wiring of biomolecules. Composite bioelectrodes by compression of enzymes and carbon nanotube mixtures will be also reported [4]. The development of glyconanoparticles resulting from the self-assembly of block copolymers composed of polystyrene and cyclodextrin as an inclusion site will be also reported [5]. These glyconanoparticles, which are stable in water, constitute a multivalent platform for enzyme binding and hydrophobic electroactive molecules. These nanoparticles were applied to the elaboration of solubilized enzymatic fuel cell in solution or were grafted on surfaces for the development of amperometric enzyme electrodes.

Key Words: Polymers, Glyconanoparticles, Nanostructured Materials, Biosensors, Biofuel Cells

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Abstract ID: 711

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Solar Cells

Keywords: Niobium oxide, Perovskite solar cells

Advances in Niobium Oxide Films for Electron Transport Layers in Perovskite Solar Cells

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Solar energy is a very promising source of renewable energy. For this reason, the scientific community is doing great efforts to improve the efficiency of photovoltaic (PV) devices and, at the same time, to reduce its costs and its environmental impact. Perovskite solar cells have attracted attention due to their high conversion efficiency and low cost. In this talk, we will present our work using Nb2O5 to improve PSCs. In the first example, niobium oxide is used as an alternative compact hole blocking layer in conjunction with mesoporous TiO2 and mixed cation Cs0,17FA0,83Pb(I0,83Br0,17)3 perovskite solar cells. It was found that an optimized Nb2O5 layer deposited by sputtering could minimize hysteresis and increase stability. The difference in performance is due to the presence of defects in the layer [1]. The influence of Nb2O5 preparation was studied and it was found to strongly influence hysteresis. Devices were constructed with 100 nm sol-gel films Nb2O5 instead of sputtered and found to have small hysteresis and low light soak effect compared with 100nm Nb2O5 sputtering deposited films. For the best device with sol-gel Nb2O5, a better option for inject printing, the energy conversion efficiency of up to 16% short-circuit currents of 24 mA/cm2 and fill factor of 64% were found. For sputtering films 18% energy conversion efficiency, short-circuit currents of 24 mA/cm2 and fill factor of 70% was observed for comparison. In addition, the use of Nb2O5 regardless of the preparation method improved the stability of the solar cells under illumination. In the second part of the talk, perovskite films were prepared in different deposition temperatures to verify the influence of grain sizes on the mobility of charge carriers. It was found that the deposition made at 31ºC resulted in films with better electrical properties which helped the extraction of the photogenerated electrons to the external circuit, improving the Jsc and consequently the device efficiency.

Key Words: Niobium oxide, Perovskite solar cells

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Abstract ID: 712

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Porous and cellular materials

Keywords: Manganese Ferrite, Chitosan Coating, Nitroarene Reduction, Allylcarbamate Deprotection

Palladium nanoparticles on chitosan-coated superparamagnetic manganese ferrite: a biocompatible heterogeneous catalyst for nitroarene reduction and allylcarbamate deprotection

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Superparamagnetic chitosan-coated manganese ferrite was successfully prepared and used as a support for the immobilization of palladium (Pd) nanoparticles. The physicochemical, morphology, and magnetic properties of the resulting Pd-supported heterogeneous catalyst (Pd_Chit@MnFe2O4) were characterized using X-ray powder diffraction, X-ray photoelectron spectroscopy, inductively coupled plasma mass spectrometry, Fourier transform infrared spectroscopy, transmission electron microscopy, field emission scanning electron microscopy and vibrating sample magnetometry. The Pd_Chit@MnFe2O4 catalyst exhibited high catalytic activity in 4-nitrophenol and 4-nitroaniline reductions, with respective turnover frequencies of 357.1 min-1 and 571.4 min-1, respectively. The catalyst can also be recovered easily by magnetic separation after each reaction. The Pd_Chit@MnFe2O4 also performed well in the reductive deprotection of allylcarbamate. Therefore, the catalytic activity of Pd_Chit@MnFe2O4 was proved to be unrestricted in biology conditions. Coating the catalyst with chitosan, reduced the Pd leaching and its cytotoxicity.

Abstract ID: 713

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: 2D materials, Salt-templated, Molten salt

Salt-Assisted Synthesis of Two-Dimensional Materials

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Two-dimensional (2D) materials have demonstrated good chemical, optical, electrical and magnetic characteristics and offer great potential in numerous applications. Therefore, corresponding synthesis technology of 2D materials with high-quality, high-yield, low-cost and time-saving is desired. This presentation will focus on the recent research progress in my group about the salt-assisted synthesis of 2D materials and their typical applications. We will discuss the properties of crystal and molten salts, provide examples of 2D materials synthesis (such as transition metal oxides, transition metal dichalcogenides, transition metal nitrides, transition metal phosphides) based on salt-templated method and molten salt method with their applications in energy storage and conversion. Importantly, the underlying mechanisms of salts with different states on the formation of 2D morphology are introduced to aid in rational synthetic route design.

Abstract ID: 714

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Epitaxial Materials and Devices

Keywords: BiFeO3, Strain engineering, Complex oxides

Strain engineering of epitaxial oxide heterostructures beyond substrate limitations

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The limitation of commercial single-crystal substrates and the lack of continuous strain tunability preclude the ability to take full advantage of strain engineering for further exploring novel properties and exhaustively studying fundamental physics in complex oxides. Here we report an approach for imposing continuously tunable epitaxial strain in oxide heterostructures beyond substrate limitations by inserting an interface layer through tailoring its gradual strain relaxation. Taking BiFeO3 as a model system, we demonstrate the introduction of an ultrathin interface layer allows the creation of desired strain states that can induce phase transition and stabilize a super-tetragonal phase as well as morphotropic phase boundaries overcoming substrate limitations. Continuously tunable strain from tension to compression can be generated by precisely adjusting the interface layer thickness, enabling the achievement of continuous O-R-T phase transition. This proposed route could be extended to other oxide heterostructures, providing a platform for creating exotic phases and emergent phenomena.

Abstract ID: 715

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Fuel Cells

Keywords: Solid oxide fuel cell, Stack, Degradation, Lifetime prediction

Durability Study and Lifetime Prediction of Solid Oxide Fuel Cells

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The present study highlights the degradation analysis and lifetime prediction of the anode-supported solid oxide fuel cells and stack. The degradation behavior of the anode-supported flat-tubular SOFCs was studied as a function of applied current load and operating temperature. The coarsening of Ni particles in Ni-cermet anode and elemental migration from cathode towards the electrolyte were diagnosed to be the major degradation mechanisms. The identified degradation mechanisms were extensively studied as a function of time and their effect on the performance degradation was evaluated. The simple mathematical models were developed to predict the performance degradation by means of cell polarization and ohmic resistance. The single degradation effects were then integrated into a comprehensive model for the lifetime prediction of the anode-supported flat-tubular SOFC stack. The experimental and modeling results exhibited reasonable agreement and provide a deep insight into the time dependent degradation of the SOFCs.

Abstract ID: 716

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Computational Electronic Materials

Keywords: Electronically conducting polymers, donor-acceptor type, intrinsic conductivity, push-pull mechanism

Recent Advances in Donor-Acceptor Type of Intrinsically Conducting and Infrared Emitting Polymers

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Impressed by the metallic conduction and superconducting behavior of poly(sulfur nitrile), also called, polythiazyl, discovered by F.P. Butt, in 1910, Alan Heeger, Alan McDirmid and Hideki Shirakawa, worked on improving conductivity of unprecedently prepared polyacetylene by exposing to iodine vapor in late 70's. These materials have extended conjugation in their polymer backbone that acts as electronic conduction path and charge carriers such as solitons, polarons and bipolarons to conduct electricity. The traditional electronically conducting polymers are (i) carbon-based ones such as polyacetylene, poly(para-phenylenevinylene), poly(azulene), heteroatomic aromatic compounds such as polypyrrole, polythiophene, polyfuran, polyaniline, their derivatives, to name a few. Most of them do not possess intrinsic electrical conduction but the conductivity could be improved by several orders of magnitude byeither p- or n-doping. Although, these polymers have a wide range of applications, their processability is very poor owing to their insolubility in common solvents, brittleness and poor mechanical properties. Some of these problems have been addressed by attaching side-chains such as long alkyl chains and alkylenedioxy groups (PEDOT) and so on. The third generation of electronically conducting polymers are the so-called donor-acceptor- (D-A) type polymers, also called push-pull polymers, where the polymer backbone consists of conjugated moieties of donor and acceptor molecules as monomer units. The commonly used donors are electron rich monomers such as thiophene, bithiophene, terthiophene, benzodithiophene, indacenodithiophene, cyclopentadithiophene and common acceptors are diketopyropyrrole, thienopyrrolodione, benzothiadiazole, 5,6-difluoro benzothiadiazole, where the acceptors are electron deficient aromatic molecules containing strongly electron-withdrawing groups. These polymers have very low band gaps capable of absorbing and emitting in the visible, near infrared and mid-infrared regions and intrinsic electronic conductivity. Functional D-A type polymers can be developed by backbone engineering and side-chain engineering. Their properties can be optimized by carefully selecting D moieties with low LUMO levels and A moieties with high HOMO levels. D-A polymers with TFT mobilities nearing or surpassing 1 cm2 V-1 s-1. The polymers have a myriad of applications in organic thin film transistors, organic photovoltaics (bulk heterojunction devices), bioelectronics, and as supercapacitors.

Abstract ID: 717

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Electrical properties of graphene, Mxenes and other two-dimensional materials

Keywords: Transition metal dichalcogenides, scanning nonlinear dielectric microscopy, local deep level transient spectroscopy

Nanoscale evaluation of carrier distribution and interface properties in atomically-thin WSe2 by scanning nonlinear dielectric microscopy

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Two dimensional (2D) semiconductors such as ultra-thin WSe2 have attracted much interest because of their intriguing material properties and semiconductor device applications. In the development of 2D semiconductor devices, understanding carrier distributions especially under external electric fields and relevant interface properties are of great importance. However, there are still limited means to investigate the nanoscale details of carrier distribution and interface properties. Here we utilized our scanning probe microscopy method called scanning nonlinear dielectric microscopy (SNDM) [1] to evaluate the differences in the electric field effects on ultra-thin WSe2 with different interface states [1]. SNDM is based on the detection of tip-sample capacitance using near-field microwave and permits nanoscale dominant carrier distribution imaging [2]. In addition, we also utilized local deep level transient spectroscopy (local DLTS) to evaluate interface defects at a nanoscale [3, 4]. Here, we compared thin WSe2 mechanically exfoliated on SiO2 and suspend WSe2. The former was as-exfoliated 3-10 layer WSe2 on a 300 nm-thick thermal oxide layer on a Si substrate. The latter was 3 layer WSe2 suspended on 40 nm-height Au wires deposited on the same substrate to avoid the strong coupling between the WSe2 layers and substrate. SNDM visualized that the as-exfoliated sample showed dc-bias dependent carrier distribution with strong hysteresis and high spatial fluctuations. We also found very high density of interface defects by local DLTS. These results imply that the as-exfoliated sample are difficult to use in transistor applications. In contrast, the suspended WSe2 showed no significant hysteresis in the carrier distribution under external dc electric fields. In addition, local DLTS showed much less interface defect density in the suspended WSe2. In conclusion, SNDM and local DLTS are useful for nanoscale evaluation of on the electric field effects and interface quality on 2D semiconductors. In addition, the suspended structure will help the improvement of the electrical characteristics of 2D semiconductor devices.

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Abstract ID: 718

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Electrical, optical, electrochemical, thermal and mechanical properties of graphene, Mxenes and other two-dimensional materials

Keywords: Graphene, Terahertz, Dirac Plasmon, PT Symmetry

Controlling the parity and time-reversal symmetry of graphene Dirac plasmons and its application to terahertz lasers

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Graphene has a unique electronic band structure that is linearly dispersed and gapless. As a result, both electrons and holes behave as relativistic charged particles of massless Dirac fermions. The quantum of plasma oscillation of these Dirac electrons is called the graphene Dirac plasmon, which can dramatically enhance the interaction of terahertz (THz) waves with graphene. We have proposed an original current-injection graphene THz laser transistor, demonstrated single-mode THz laser oscillation at low temperatures1-3), and discovered and demonstrated the THz giant gain enhancement effect by graphene Dirac plasmons4,5). However, in order to realize room temperature high intensity THz lasing and ultrafast modulation operation, which are necessary for the next generation wireless communication of 6G and 7G, further breakthroughs are needed. In this work, we introduce completely new physics and principles to simultaneously break through the limits of quantum efficiency and high-speed modulation operation by actively controlling the parity and time-reversal symmetry6) of graphene Dirac plasmons with nanostructures and applied voltages. In this talk, we will present new ideas on the operating principle and device structure of graphene plasmonic laser transistors with high radiation intensity and ultrafast modulation capability operating at room temperature in the THz frequency band.

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Abstract ID: 719

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Phase Change Materials

Keywords: Light-induced phase transitions, ultrafast time-resolved spectroscopy, phase-change materials, femtosecond laser-induced processes

Ultrafast time resolved pump-probe study of the phase transition's kinetics in transition metals chalcogenides induced by femtosecond laser radiation

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Due to a high optical and electrical contrast in the two stable phase states, switched by the impact of laser radiation [1], transition metal chalcogenides such as GeTe, GeSbTe, GeSbSeTe are of great interest to researchers as materials applicable in high-speed photonic and optoelectronic devices, as well as a functional material for developing basic elements of optical multivalued logic and neuro-inspired logical and memory devices, for example, optical synapses and universal memory devices [2]. The use of ultrashort laser pulses of femtosecond duration technique for induced phase transformation opens possibilities of studying ultrafast processes of crystallinity change [3] and carrier dynamics [4] during phase transition. Also, femtosecond pulse laser radiation is more effective in inducing crystallization of chalcogenides thin films than the nanosecond pulse laser radiation [5]. This paper presents the results of a study of phase light-induced phase transitions in samples of thin films of the above materials on various substrates in a high-resolution pump-probe spectroscopy using femtosecond laser radiation on a laboratory setup that we demonstrated in our previous works [1, 6] and modified taking into account the temporal resolution and the use of an ultrashort pump source [7].

Key Words: Light-induced phase transitions, ultrafast time-resolved spectroscopy, phase-change materials, femtosecond laser-induced processes

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Abstract ID: 720

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: graphene nanoribbon, on-surface synthesis, bandgap, scanning tunneling microscopy, non-contact atomic force microscopy

On-surface synthesis of small bandgap graphene nanoribbons

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Graphene nanoribbons (GNRs), quasi-one-dimensional strips of graphene with atomically precise width, exhibit unique electronic and magnetic properties depending on the edge structure and width of the GNRs. Armchair-edged GNRs (AGNRs) with finite bandgaps have attracted much attention for their potential reliability as organic semiconducting materials. After the first report of bottom-up synthesis of anthracene GNR (7-AGNR, where 7 is the width measured by the number of rows of carbon atoms across the AGNR) by on-surface-assisted polymerization and subsequent cyclodehydrogenation of precursor monomers on metal surfaces in 20101, many attempts have been reported to control the bandgap of AGNRs by the edge modification, control of the ribbon width, and the insertion of heteroatoms to AGNRs.

From theoretical calculation, the wider AGNR was predicted to have smaller bandgap size. We started with the synthesis of bis-diketone precursor of 7,16-dibromo-heptacene for the on-surface synthesis of 15-AGNR, but heating of the precursor on Au(111) surface offered hepta-cene organometallic complex instead of 15-AGNR.2 The steric hindrance between precursors prevented the polymerization of the precursors and gold atoms were inserted between the mon-omers. In 2020, we were successful in the first on-surface synthesis of 17-AGNR using 1,2-bis-(2-anthracenyl)-3,6-dibromobenzene as a monomer and in characterization of 17-AGNR by combining in situ scanning tunneling microscopy and spectroscopy (STM/STS) and ex situ non-contact atomic force microscopy (nc-AFM).3 We revealed that the 17-AGNRs have a bandgap of 0.19eV on Au(111), which is consistent with a theoretically obtained bandgap of 0.63 eV for a freestanding 17-AGNR.

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Abstract ID: 721

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Magnetic Polymer

Keywords: Soft elastomers, Magnetic microparticles, Dynamically responsive composites

Magneto responsive surfaces for manipulation of light and liquids

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Magnetoactive elastomers (MAEs) are rubbery substances composed of a soft polymer matrix with embedded micrometer-sized ferromagnetic particles. They are also known as magnetorheological elastomers (MREs) and are often perceived as solid analogues to magnetorheological fluids. Hitherto, the majority of research on MAEs was concentrated on their bulk properties. However, recently it has been realized that surface properties of MAEs substantially alter in a magnetic field too, which opened a new emerging research field associated with them. The main underlying mechanism of magnetically tunable surface properties of MAEs are magnetic field-induced modifications of their surface roughness. Due to this property, MAEs are an excellent candidate for magneto responsive surface coatings with dynamically tunable characteristics. We investigated the effect of an external magnetic field on the splashing behavior of ethanol drops impacting on the surface of soft MAEs. The Weber number corresponding to the transition between the deposition and the splashing regime decreases with increasing magnetic field. Alongside this effect, a significant increase of the initial deceleration of the ejection sheet also takes place. We studied also the effect of magnetic field on reflection of laser light from a MAE surface. With increasing magnetic field, the specular reflection is transformed to spread reflection. Moreover, the total reflectivity from the surface is also strongly reduced.

Acknowledgements

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Abstract ID: 722

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Electrical properties of graphene, Mxenes and other two-dimensional materials

Keywords: ARPES, MBE, transition metal dichalcogenides, two-dimensional materials

Electronic structures of epitaxially-grown atomically-thin transition metal dichalcogenides

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Atomically-thin two-dimensional (2D) materials often exhibit novel physical, chemical, and optical properties that are largely different from their bulk counterparts. These properties are governed by the changes in the band structure and the lattice symmetry, and most pronounced in their single layer limit. Angle-resolved photoemission spectroscopy (ARPES) is a direct tool to investigate the underlying changes of band structure to provide essential information for understanding and controlling such properties. We have been utilizing ARPES on atomically-thin 2D layers of transition metal dichalcogenides (TMDC) grown on bilayer graphene substrate using molecular beam epitaxy (MBE). Distinct electronic and topological properties of these 2D films, such as indirect-direct band gap transition [1], charge density wave order [2], and topological phase transitions [3], will be discussed.

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Abstract ID: 723

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Solar Cells

Keywords: Passive intelligence, multi-functional BIPV, Bi-facial PV module, Building energy conservation.

Theoretical Optimization of bi-facial BIPV Module for Apartment

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Theoretical Optimization of bi-facial BIPV Module for Apartment

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There are many kinds of technologies to mitigate greenhouse gases for a sustainable world. The largest portion of greenhouse gases comes from the building sector, especially in developed countries. In Korea, all new public buildings (Total floor area: 1,000㎡↑) by 2020 and all buildings (Total floor area: 500㎡↑) by 2030 should be built as a near-zero energy building to mitigate greenhouse gasses in the building sector. The theme of this research is to ecologically supply nearly zero-energy solar architecture with minimal cost by suggesting the optimal energy harvesting methodologies, multi-functional BIPV, reasonable building envelope concepts, considering the regional climate and architectural culture of the corresponding climate zone combined to bi-facial BIPV module system.

This research is mathematically analyzed to make an ecological PV envelope system or design criteria close to a zero-energy building, as a kind of multi-functional building integrated photovoltaic (BIPV) which bi-facial BIPV modules are deployed to passive solar concepts, to minimize the heating & cooling load, to upgrade the indoor environmental quality, and to be adjustable for regional climate, and to continuously succeed architectural culture and history through optimization of element technologies including any possible system based on natural energy resources, to fundamentally mitigate climate change and indoor environment.

The concept and design criteria for the nearly zero-energy solar architecture of this research are focused on the ecological use of bi-facial PV modules. How to maximize solar gain in the heating period, how to eliminate solar irradiance outside the building envelope in the cooling period, and how to maximize power generation by bi-facial BIPV module could be the most important interest for this research. This multi-functional BIPV concept of bi-facial PV module as a shading device could be also ecologically nice PV technology with the passive intelligent system concept in an eco-friendly and effective manner while improving the human comfort in a building and drastically reducing the cooling load of a building, especially in a hot or temperate climate zone.

Key Words: Passive intelligence, multi-functional BIPV, Bi-facial PV module, Building energy conservation.

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Abstract ID: 724

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Solar Cells

Keywords: Electrical bistablity, CdZnTe thin films, C-AFM.

Electrical Bistablity studies on D.C sputtered CdZnTe (CZT) Thin films

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CdZnTe thin films were fabricated on glass substrates by D.C Sputtering Technique. X-ray diffraction pattern confirms the presence of Zinc blende CZT (CdZnTe), whereas the Scanning electron microscopic (SEM) analysis shows the 1-D morphology of the CZT (CdZnTe) films. Electrical studies shows the bistability phenomena of CZT (CdZnTe) films. The current-voltage (I-V) characteristics showed two distinct paths for forward and reverse sweep directions. Conducting Atomic Force Microscopy (C-AFM) studies also supported the bistability phenomena of the CdZnTe films. Current investigations on electrical bi-stability of the CdZnTe thin films will help to understand the defects in the photo absorber materials and the PV performance of the CdZnTe based device.

Abstract ID: 725

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: Catalysis, Bismuth nanoparticles, Trimethyl Chitosan, Chitosan

Synthesis of Bismuth Anchored Quaternary Trimethyl Chitosan Nanocomposites as Smart System for Catalysis

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One of the critical challenges facing modern society is conversation wastes to renewable, eco-friendly, socially acceptable, economically competitive and sustainable liquids. Bismuth-based nanoparticles are unique category of materials that possess interesting properties such catalytic activities, excellent chemical, electrical and optical activities among other. The application of bismuth-based nanoparticles as photocatalytic materials has caught the interest of the scientific community in recent time due to these unique properties. In this study, a quaternary water-soluble cationic chitosan derivative, N,N,N-trimethyl chitosan (QTMC) was synthesized via two-step reductive methylation of Chitosan (CTS). The new biopolymeric functionalized ligand was further used as capping agent for the synthesis of bismuth nanoparticles (QTMC-BiNPs). The concentration effect of saccharide unit of polymeric N,N,N-trimethyl CTS on the particles size and formation yield of QTMC-BiNPs were also investigated. The Degree of Quaternization (DQ %), Degree of Dimethylation (DD %) and aqueous solubility saturation of QTMC were determined and compared with the native CTS. In addition, the CTS, QTMC and QTMC-BiNPs were fully characterized by spectroscopic methods (Proton Nuclear Magnetic Resonance Spectroscopy, Attenuated Total Reflection Fourier-Transform Infrared Spectroscopy, Ultraviolet-Visible Spectroscopy, X-ray Diffraction, Energy Dispersive X-ray Spectroscopy, Selected Area of Electron Diffraction and X-ray Photoelectron Spectroscopy), Microscopic methods (Scanning Electron Microscopy and High Resolution Transmission Electron Microscopy) and Thermogravimetric Analysis/Derivative Thermogravimetry. The catalytic performance of QTMC-BiNPs for the reduction of 4-nitrophenol (4-NP) to 4-aminophenol (4-AP) in the presence of sodium borohydride was studied. The degree of reusability of the catalyst and time dependent reduction of 4-NP to 4-AP were also investigated. The catalytic activity of QTMC-BiNPs is very promising and hence could be considered as high-performance catalyst for the conversion of 4-NP to 4-AP.

Abstract ID: 726

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Electrochemical Supercapacitors

Keywords: Carbon, Supercapacitor, Pseudocapacitance, Energy Storage

Tailoring Biomass Carbon for High Density Charge Storage

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Emergence of sustainability as the new normal and consequent concerns over materials sustainability for various industrial sectors accelerated materials discovery process from renewable sources [1]. Energy storage become one of the dominant industries currently and most of the high performing energy storage devices such as lithium ion batteries use expensive mined materials as electrodes with enormous processing and value addition. Biomass derived carbon has been suggested as a possible material for energy storage, however, they mainly suffer from lower performance indicators [2 -3]. We have explored augmenting properties of biomass carbon with small amounts (~5 – 10 wt.%) of metals or metal oxides to enhance the charge storage parameters in lithium ion capacitors, battery – supercapacitor hybrids, and symmetric supercapacitive storage modes. Three strategies were adopted: (i) enhancing the charge storage sites by filling large voids in porous carbon by hierarchical 3D nanoflowers or composite nanostructures [4-6], (ii) developing a thin metal oxide film over porous carbon surface through a simultaneous activation and coating process [7], and (iii) developing a thin metal film over porous carbon [8]. All these protocols have developed carbon composite electrode with several folds higher charge storability without losing their advantage on higher specific power. Three types of laboratory prototypes operating in lithium ion capacitors, battery – supercapacitor hybrids, and symmetric supercapacitive storage modes were developed using these electrodes in aqueous as well as nonaqueous electrolytes with voltage up to 3.5 V. The best performing device was a BSH of maximum specific energy of ~153 Wh·kg-1 and maximum specific power ~3500 W·kg-1 employing 3-dimensional $MnCo_2O_4$ nanoflowers (3DMCNF) battery-type anode and a carbon electrode containing 3DMCNF (M3DMCNF) as supercapacitor-type cathode in 1 M $LiPF_6$ electrolyte.

Keywords: Carbon, Supercapacitor, Pseudocapacitance, Energy Storage

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Abstract ID: 727

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: CCS, Device, H2 sensing

Role of carbon Materials in Hydrogen Gas Sensing Application

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The development of gas sensors for the detection of toxic gases like NH3, CO and H2 existing in the atmosphere. Among these gases, H2 is odorless, colorless and flammable at concentrations greater than 4%. However, H2 is explosive over the range of 15% at standard atmospheric temperature. H2 gas is predictable to be extensively used as an energy source for fuel cells and it has wide applications in civil transportation. Therefore, H2 gas sensor is necessary to ensure safe operation of hydrogen based energy storage systems and facilities such as H2 gas stations, fuel cell based vehicles, semiconductor manufacturing and in rockets for space vehicles, since H2 leakage leads to explosive accidents. To shun this accidents, H2 gas sensors have been developed using carbon nanotubes (CNTs), Graphene, Carbon nnaomaterials, carbon horn and their nanostructures with metal/metal oxides nano-particles. However, in the present work, the inexpensive candle carbon soot (CCS) is used to detect 0.5% concentration of H2 gas at room temperature. A simple flame of candle is used to synthesize the layers of carbon soot at room temperature conditions. It is observed that, the acid treatment of CCS drastically improved their structural and sensing properties as compared to as-synthesized CCS. The effect of acid functionalization on the CCS structure were investigated by X-ray diffraction (XRD) and Raman spectroscopy. To the best of our knowledge, detection of low concentrations of H2 gas is reported here for the first time using economical CCS at room temperature. These results are important for developing a new class of chemiresistive type gas sensor based on change in the electronic properties of the CCS.

Abstract ID: 728
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Nanocomposites
Keywords: Layer-by-Layer, SERS, AgNPs, Diatom, Nanocomposite

Layer-by-Layer Assembly of Silver Nanoparticles on Diatom Frustules for Surface-enhanced Raman Scattering

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Surface-enhanced Raman Scattering (SERS) is an emerging analytical technique used for characterization of biological and non-biological structures. Plasmonic properties of nanostructures are main factors influencing SERS performance. Thus, fabrication of plasmonic nanostructures having different plasmonic properties is a significant research interest. Recently, guided-mode resonances (GMRs) in diatoms have significant attention due to their potential contribution to SERS enhancement. Furthermore, there is also evidence showing that diatoms can be utilized in improving SERS enhancement by optically coupling the GMRs of the diatom frustules with the LSPRs of the nanostructures. In this study, inexpensive, robust, and flexible diatom-based SERS platforms having different number of layers on a box tape are fabricated using layer-by-layer assembly of silver nanoparticles (AgNPs). The fabricated SERS platforms are characterized using UV-Vis spectroscopy and scanning electron microscopy (SEM). The SERS performance of the platforms was evaluated using 4 aminothiophenol (4-ATP) and rhodamine-6G. The results demonstrate that SERS performance of the platforms is dependent on the number of layers of the structures. The SERS platform having highest SERS activity can be used for the characterization of any molecules of interest

Abstract ID: 729

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanomaterials and Nanotechnology

Keywords: Nanodomes, Nanovoids, Nanocomposites, Bacteria, Protein

Label-Free Biosensing on Plasmonic Nanostructures Using SERS

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Surface-enhanced Raman scattering (SERS) is an emerging analytical technique for the detection and identification of chemicals and biological molecules and structures. Rapid, sensitive and accurate identification of biomolecules and structures is critical not only clinical diagnostics but also industrial applications. Several studies have been demonstrated that SERS can be used as powerful technique for the identification of bacteria and proteins using different sample preparation methods and SERS substrates. Sample preparation and SERS substrates are critical factors to obtain strong, sensitive, and reproducible SERS spectra from the analytes. In this study, label-free identification and characterization of bacteria and proteins on different plasmonic nanostructures is demonstrated. Different types of SERS substrates (plasmonic nanovoids and nanodomes and nanocomposites) are fabricated using different fabrication approach and characterized. Different types of bacteria and proteins are used to test the performance of the fabricated plasmonic nanostuructures for SERS-based biosensing.

Abstract ID: 730

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Ferroelectricity and piezoelectricity

Keywords: Multiferroic, elastic properties, pump-probe method

Elastic properties assessment in the multiferroic BiFeO3 by pump and probe method

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Multiferroics that show cross-correlation between electric and magnetic properties are promising materials for future hybrid computational architectures that transform information from one state into another, such as spin excitations into charge, phonons or photons. Among multiferroics, bismuth ferrite (BiFeO3) is the prototypical multiferroic with outstanding properties and has shown application potential in fields as diverse BFO-based nanoelectronic devices and spintronic. It leads also to spectacular THz electromagnetic wave generation and photostriction properties. The prospects for applications in this area such as optically triggered piezotransducers require a perfect knowledge of the elastic properties of materials. The knowledge of the elastic properties of BFO is desired for the integration of BFO in nano-electronic devices.

Combining pump-probe experiment at the picosecond time-scale with density functional theory and calculations of theoretical velocities, all the Cij elastic constants have been determined in an unprecedented effort.1 Our methodology necessities only one single crystal whereas more are needed in case of Brillouin scattering.

We implement pump-probe experiment at the picosecond time-scale on BFO single crystal to measure the sound velocities of the (quasi)-longitudinal and two (quasi)-transverse acoustic waves along three independent directions of the (110) surface. Moreover, one surface wave and one longitudinal wave propagating perpendicular to the surface have been detected.

From a set of initial elastic constants calculated by the density functional theory, the resolution of the Christoffel equation gives access to first theoretical velocities. The minimization of the difference between the experimental and theoretical velocities allows determining all six independent Cij elastic constants. The comparison of the directional dependency of experimental and theoretical sound velocities enables identification of the longitudinal, fast and slow transversal acoustic modes and the generalized Rayleigh surface wave.

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Abstract ID: 731

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Graphene, Mxenes and other two-dimensional materials for biomedical and healthcare applications

Keywords: Antimicrobial, 2Dnanomaterial, nano Surface

New Perspectives on Drug-Free Antimicrobial/ Antibiofilm Mechanisms Enabled by 2D Nanomaterial Surfaces

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Novel 2D nanopatterns exhibit antibacterial properties which may be implemented in antibacterial, antimicrobial,or anti-odor materials, including fibers, clothing, medical supplies and other surfaces, such as bandages. This project aims to produce a fundamental and mechanistic understanding of the mechanism by which 2D nanopatterns may kill bacteria. This fundamental understanding will allow improvement the conventional and current antibacterial treatments that are based on biochemical antibiotic drug mechanisms. Such physical and fast acting antimicrobial mechanisms are not limited to nanopatterned surfaces or specific strain of bacteria. They are rather generalizable to a broad spectrum of bacterial strains. Conventional antibacterial treatments fail due to bacterial adaptation, high costs, and the repeated application required by chemical treatments. Antibacterial products containing conventional antibacterial treatments function by releasing the antibacterial agents slowly over time, which leads to eventual exhaustion of the antibacterial treatment and limits the lifespan of the product. In contrast, novel 2D nanomaterials represent a fundamentally different approach, which may prevent bacterial adaption and do not require continuous reapplication. Novel 2D nanosurfaces were synthesized for drug free antibacterial treatments. Such Nano surfaces allow new biomedical applications of drug-free antibacterial treatments as liquids, gels, powders or coatings on the surface of implants. Our results suggested the bactericidal mechanism occur due to direct penetration and deformation of the cell wall as opposed to biochemical mechanism of antibiotic drugs. In addition such fast and direct mechanism will not allow enough time for the bacteria to communicate and therefore may prevent the formation of biofilm and infection. Conclusions: Fundamental and mechanistic understanding of the mechanism by which nanopatterns may kill bacteria were produced suggesting that the bactericidal mechanism of nanopatterns occur due to physical mechanism of direct penetration of the bacterium and deformation of the cell wall as opposed to chemical mechanism of antibiotics This fundamental understanding will allow improvement of the current antibacterial treatments, enabling a fast “touch and kill” antimicrobial effect by physical stabbing of the bacteria via nanopatterns. Interestingly is the generalizability of this method to a broad spectrum of bacterial strains.

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Abstract ID: 732

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Optical properties of metals and non-metals

Keywords: Graded, Photonic system, linear index profile, quadratic index profile

Optical properties of 1D graded photonic crystals considering linear and quadratic profiles

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By using the transference matrix formalism, in this work it is presented the study of the optical properties of 1D photonic structures constructed by M periods of bilayers of dielectric material and slabs with graded index profile of two types: linear and quadratic. By varying the profile parameters, while it is preserved the average value of the refractive index for the graded slab, it is compare and describe the formation of new photonic band gaps for which its bandwidths depends on the slope and the curvature of the linear and quadratic profile respectively. Also, it is found the formation of omnidirectional photonic band gaps for the TE and TM polarization, one for the linear profile and three for the quadratic one, for which their bandwidths depends linearly on the slope and the curvature of the graded profiles. It is expected that the presented results could be useful in the construction of optical devices based in their optical response under oblique incidence.

Abstract ID: 733

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Optical properties and spectroscopy of graphene and other two-dimensional materials

Keywords: transition metal dichalcogenides, quantum defects

Creation of quantum defects in transition metal dichalcogenides for quantum photon source applications

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Recently, quantum defects in transition metal dichalcogenides (TMDs) have been discovered as efficient single-photon sources. Coupled with the atomic layer thickness, distinct optoelectronic properties, and strong spin-valley locking of TMDs, quantum emitters in TMDs constitute a compelling platform for generating single photons. Here, we demonstrate an approach for creating quantum defects in TMD monolayers through strain engineering. Utilizing the nanometer-sized sharp tips of gold nanostars, we are able to create local strain profiles with a sub-10 nm spatial precision and observe single photon emission from the created quantum emitters.[1] Moreover, our analysis of the defect emission characteristics reveals the associated strain types that create the defects. We further apply the strain engineering approach to interlayer excitons in TMD heterostructures and observe strikingly different photophysics from the intralayer excitons.[2] These findings could help the precise creation of quantum defects in TMDs and deepen current understanding of their electronic structures.

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Abstract ID: 734

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Bio-inspired design of composites

Keywords: Cellulose nanocrystas, photocatalysis, Sol-gel, TiO2

Cellulose nanocrystals: a sustainable biotemplate for highly active and mesostructured photocatalyst

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Solar energy conversion using photocatalysis becomes a subject of great interest with important potential applications in environment, such as chemical fuel production (H2).[1] [2] [3]Titanium dioxide (TiO2) is the most popular semiconductor used in photocatalysis. However, TiO2 has a large band gap and can only be excited by UV light. Furthermore, the fast recombination of electron-hole pairs lowers the solar energy conversion efficiency. Design of the photocatalyst in 3D structure appears as a promising strategy to increase the ligth harvesting and the photogeneration of electron/hole charges.[4] [5] In this aim, cellulose nanocrystals (CNC) was combined to sol-gel chemistry for one-pot elaboration of lamellar photocatalysts. This enables the improvement of light harvesting ability of the material by multiple ligth scattering. Evaporation-induced self-assembly (EISA) method produces iridescent hybrid films in which the chiral nematic arrangement of CNC is preserved. The morphological, textural and structural properties of the final photocatalysts were characterized by SEM, BET, POM, TRMC, WAXS. The effect of the CNC/TiO2 ratio as well as coupling the photocatalyst with nanopartilces based on abundant metals were evaluated for hydrogen generation. We found that structuration of the photocatalyst and its modification with non-nobel metal nanoparticles enhance light harvesting, charge carriers density and separation reaching higher photon to energy convertion.

Abstract ID: 735

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Polymeric composites

Keywords: light harvesting, conjugated polymer, polyelectrolyte, self-assembly, water

Towards Mimicking Light-Harvesting Organelle Function with Water-Soluble Conjugated Polymers

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The ability to assemble complex, artificial light-harvesting systems that mimic natural light-harvesting organelles in water is both fascinating and attractive from a practical point of view. The components of such a system must be capable of self-assembly and strong light absorption. They must also support rapid transport of photogenerated electronic excited states (excitons) through space to ensure that few photons are wasted. Excitons must then be converted to electron/hole pairs that live long enough to drive chemical reactions. Conjugated polyelectrolytes (CPEs) combine several characteristics that make this materials class a promising foundation for this application. Using these materials, we are focusing on associative phase separation of CPEs as a means to form membrane-less light-harvesting organelle mimics. We have shown that associative phase separation can form complex coacervate-like concentrated CPE fluids with photophysics that can be manipulated with simple ions via the cation-pi interaction. Our recent work shows that molecular ions can stabilize concentrated phases that contain an exciton donor/acceptor CPE network with properties reminiscent of dense fluids and hydrogels. In parallel, we are also working on constructing hierarchical membrane-based panchromatic systems based on soft macroion vesicle scaffolds. To form an exciton and electron cascade that forms long-lived electron/hole pairs, we aim to simultaneously take advantage of both the outer and inner membrane/water interfaces, along with the hydrophobic membrane interior. I will discuss our current progress in forming self-assembled, directional exciton funnels oriented from outside towards the membrane interior.

Abstract ID: 736

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Ferroelectricity and piezoelectricity

Keywords: piezoelectric, nanofiber, electrospinning, bio-application

Transformative piezoelectric enhancement of electrospun P(VDF-TrFE) by nanoscale dimensional reduction and their potential bio-applications

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Despite the significant potential of organic piezoelectric materials in the electro-mechanical or mechano-electrical applications that require light, flexible, and biocompatible materials, the intrinsically low piezoelectric performance as compared to traditional inorganic materials has limited their full utilization. We demonstrate that dimensional reduction of poly(vinylidene fluoride trifluoroethylene) (P(VDF-TrFE)) at the nanoscale by electrospinning, and furthermore with an appropriate thermal treatment, induces a transformative enhancement in piezoelectric performance. Specifically, the piezoelectric coefficient (d33) reached up to -108 pm/V, approaching that of inorganic counterparts. Electrospun mats composed of these thermo-treated 30 nm nanofibers with a thickness of 15 μm produced consistent peak-to-peak voltage of 38.5 V at a strain of 0.26%. This exceptional piezoelectric performance was realized by the enhancement of piezoelectric dipole alignment and the materialization of flexoelectricity, both from the synergistic effects of dimensional reduction and thermal treatment. Our findings suggest that dimensionally controlled and thermally treated electrospun P(VDF-TrFE) nanofibers provide an opportunity to exploit their flexibility and durability for mechanically challenging applications while matching the piezoelectric performance of brittle, inorganic piezoelectric materials. By fine tuning their properties, we demonstrate their potential applications pertaining to nano-biotechnology/medicine in drug release, nerve regeneration, and a wearable device.

Abstract ID: 737

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Electromagnetic radiation

Keywords: Sic, CFRP, Antenna, Terahertz

Terahertz Antennas Using thermally stable Materials

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There are special demands for antennas used in terahertz remote sensing. In particular, a high beam efficiency is required to achieve the necessary contrast for the scene-brightness variation. With the frequency increasing to terahertz, the accuracy of antenna surface is required much more rigorously. As is known to all, it is very difficult to reach several micros root-mean-square (RMS) surface accuracy using relatively “soft metal” such as alumina for the possible space use. Contrary to the conventional metal reflectors, the dishes consisting of thermally stable carbon fiber-reinforced plastic (CFRP) sandwich structures and silicon carbide (SiC) can achieve much higher RMS surface accuracy. These two typical materials mentioned above can be found in the application of terahertz antenna. Another hurdle existing in the measurement of the THz antenna for the application of remote sensing is that since the antenna aperture is electrically large, an indoor near field system would capable of testing the same size aperture, near-field range system spends more test time than compact rang for simple pattern cut measurements. The cryo-temperature experiment can imitate the real space surroundings, which provides convenience for antenna measurement. In this paper, the large aperture high gain antenna patterns are analyzed by physics optics software based on the optical test data.

Abstract ID: 738

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nano-Magnetic, Magnetic Memory and Spintronic Materials

Keywords: Spin orbital torque, Dzyaloshinskii-Moriya interaction(DMI), Ferroelectric

Spin-orbitronics in the ferromagnetic metal/ferroelectric interface

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Spin orbit interaction (SOI) plays a key role in recent explorations to achieve high density and energy efficient spintronic devices, such as the perpendicular magnetic anisotropy (PMA) of ferromagnetic metal for memory application, Dzyaloshinskii-Moriya interaction (DMI) and current-induced spin-orbit fields for magnetization manipulations. These phenomena are normally discussed at interfaces between the ferromagnetic metal and oxide (or heavy metal), which also provides another important ingredient for them, broken inversion symmetry at the interface. With the presence of the extra degree of freedom provided by the functional ferroelectric oxide, the ferromagnetic metal/ferroelectric interface can be an interesting platform to investigate these SOI-based phenomena. In this presentation, we will present our recent exploration on this functional interface. First, we report on the study of both PMA and DMI at the ferroelectric oxide/ferromagnetic metal interface, i.e. BaTiO3 (BTO)/CoFeB. Thanks to the functional properties of the BTO film and the capability to precisely control its growth, we are able to distinguish the dominant role of the oxide termination (TiO2 vs BaO), from the moderate effect of ferroelectric polarization in the BTO film, on the PMA and DMI at the oxide/FM interface. We find that the interfacial magnetic anisotropy energy of the BaO-BTO/CoFeB structure is two times larger than that of the TiO2-BTO/CoFeB, while the DMI of the TiO2-BTO/CoFeB interface is larger.[1] We explain the observed phenomena by first principle calculations, which ascribe them to the different electronic states around the Fermi level at the oxide/ferromagnetic metal interfaces and the different spin-flip process. Second, we present a pathway to tune the effective magnetic field by engineering the Rashba effect in the BaTiO3/CoFeB/Pt structure [2]. The polarizations of BaTiO3, either up or down, are controlled by the interface engineering. The current-induced effective magnetic fields increase by more than 200% when the ferroelectric polarization of BaTiO3 changes from up to down. The changes in the effective magnetic field are mainly attributed to the different Rashba effective fields induced by the opposite ferroelectric polarizations.

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Abstract ID: 739

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Point Defects, Doping and Extended Defects

Keywords: Single Atom Alloy, Pd Doping, PdCu, Infrared Spectroscopy, Hydrogen Activation

Propyne Hydrogenation over a Pd/Cu(111) Single-Atom Alloy Studied using Ambient Pressure Infrared Spectroscopy

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The hydrogenation of propyne (C3H4) to propene (C3H6) using a Pd/Cu(111) single-atom alloy (SAA) has been studied using polarization-dependent reflection absorption infrared spectroscopy. This method allows for simultaneous monitoring of reactants and products in the gas phase and species adsorbed on the surface during the reaction. The results were compared with the hydrogenation of propyne using Pd-free Cu(111) as well as with previous studies on Pd/Cu SAA catalysts supported on alumina. Propene production occurs at temperatures of 383 K and above as indicated by the appearance of an infrared peak at 912 cm–1, which is a unique characteristic feature of gas phase propene. Propyne was found to adsorb on the surface at 300 K in the presence of gas phase propyne to form a di-σ/di-π structure, as the spectrum was identical to that reported in the literature for propyne adsorbed on Cu(111) at 150 K in ultrahigh vacuum. The presence of a carbonaceous layer on the surface is indicated by a dramatic increase in the intensity of a peak at 2968 cm–1 at temperatures above 400 K. The progression of gas phase peaks at 912 and 3322 cm–1 was used to calculate the rate of production of propene and the rate of consumption of propyne, respectively. This reaction rate was used to determine a turnover frequency of 25.4 s–1 at 383 K for the reaction on the Pd/Cu(111) SAA surface. The reaction was not impeded by the presence of the carbonaceous layer, even for a layer so thick that only carbon was detectable on the surface with Auger electron spectroscopy.

Abstract ID: 740

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Industrial applications of composite materials

Keywords: Bracing system, Polyurethane, Self-centering, Experimental testing

Development of a Novel Polyurethane-based Self-Centering Bracing

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In braced frames, the response of a structure after an earthquake can be affected by the bracing system's strength and properties. Concentric Braced Frames (CBFs) are mostly used to resist the seismic load. However, traditional tension-compression bracing system may not perform well under earthquake loads because of buckling in compression. Among other bracing systems, e.g., Buckling Restrained Bracings (BRBs) are being used to resolve this issue and help resist seismic loads. However, they cannot prevent permanent deformation in the building. To overcome the shortcomings of the developed system, a new Polyurethane Piston Based Bracing (PPBB) system has been developed and fabricated at the Applied Laboratory for Advanced Materials & Structures (ALAMS) at UBC. This device consists of a brace system that can take a considerable tension and compression force. The system is a cylinder-piston assembly in which polyurethane and steel are utilized. This specimen consists of five main parts: two halves of steel tubes, two polyurethane cylinders, and a shaft. Quasi-static as well as strain rate experimental tests were performed on the device where very good self-centering behavior was achieved using this relatively cheap and light material.

Abstract ID: 741

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: Graphene oxide; CeO2-ZrO2; Nanocomposite; anticorrosion coatings; hydrophobic surface; Interfacial interaction

Fabrication of ceria-zirconia decorated graphene oxide for obtaining a high performance epoxy nanocomposite film with excellent anti-corrosion/mechanical properties

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This research focuses on the synthesis and modification of graphene oxide (GO) nanosheets with ceria-zirconia hybrid nanoparticles. The main aim is to take the advantages of both graphene oxide and ceria-zirconia in enhancing the long-term performance of nanocomposites. For this purpose, the synthesized graphene oxide was treated with ceria-zirconia hybrid nanoparticles. The modified GO hybrid nanosheets were characterized by Fourier transform infrared spectroscopy (FTIR), Field Emission scanning electron microscopy (FE-SEM), X-ray diffraction analysis (XRD), Ultraviolet–visible spectrophotometry (UV–Vis) and Raman spectroscopy. The effects of intercalation of GO sheets, CeO2-ZrO2 and GO/CeO2-ZrO2 nanohybrids on the corrosion protection and barrier performance of the epoxy coating on mild steel were also investigated in natural seawater by electrochemical impedance spectroscopy (EIS) and scanning electrochemical microscopy (SECM). The optimum percentage of ceria-zirconia embedded GO nanoparticles in the epoxy coating (unmodified and triazole modified) was 1.0 wt% in which the coating has minimum agglomeration and appropriate corrosion resistance. The EIS data indicated that the coating resistance of epoxy/CeO2-ZrO2 hybrid nanoparticles-modified GO after 480 h immersion in natural seawater is higher than epoxy/unmodified GO nanosheets. SECM analysis confirmed that the dissolution of Fe2+ was suppressed at the scratch on the coated mid steel due to the higher resistance for anodic dissolution of the substrate. The water contact angle (WCA) results confirmed the reduction of the hydrophobic nature of the surface after the incorporation of GO/ CeO2-ZrO2 hybrids. SEM/EDX analysis showed that Ce and Zr were enriched in corrosion products at a scratched area of the coated steel after corrosion testing. FIB-TEM analysis confirmed the presence of the nanoscale oxide layer of Ce and Zr in the rust of the steel, which had a beneficial effect on the corrosion resistance of coated steel by forming protective corrosion products in the wet/dry cyclic test. The improved mechanical properties were noticed for the nanocomposite coatings containing CeO2-ZrO2 hybrid nanoparticles-modified GO nanosheets.

Abstract ID: 742

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Nanostructured materials for advanced batteries

Keywords: Shape Memory Effect, Martensitic Transformations, Energy Storage, Lattice Twinning and Detwinning.

Phase Transformations and Energy Storage in Shape Memory Alloys

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Shape memory alloys take place in class of smart materials, due to the shape reversibility and capacity of responding to changes in the environment. These alloys exhibit a peculiar property called shape memory effect, which is characterized by the recoverability of two certain shapes of material at different temperatures. This phenomenon is initiated by thermostatically treatments and performed by heating and cooling after these treatments in bulk level. These alloys are deformed plastically in low temperature condition; strain energy is stored in the material and released on heating by recovering original shape; and shape of the materials are cycled between original and deformed shapes. Stressing and releasing paths are different at the stress-strain diagram and this result refers to energy dissipation. This effect is based on successive thermal and stress induced martensitic transformations, which occurs on cooling and stressing in atomic level. Thermal induced transformations are exothermic reactions and occur along with lattice twinning on cooling, and ordered parent phase structures turn into twinned martensitic structure. Twinned structures turn into detwinned martensite by means of stress induced martensitic transformation by stressing material. Shape recovery is performed by endothermic austenitic transformation on heating and detwinned martensite structures turn into the ordered parent phase structure. Thermal induced martensitic transformation occurs with the cooperative movement of atoms in <110 > -type directions on {110}-type planes of austenite matrix by means of lattice invariant shear. Forward martensitic and reverse austenitic transformations are solid state reactions, and these reactions do not occur at the equilibrium temperature at Gibbs Free Energy Temperature Diagram and a driving force is necessary for the transformations.

Copper based alloys exhibit this property in metastable β-phase region, which has bcc-based structures; lattice invariant shears are not uniform in these alloys, and the ordered parent phase structures martensitically undergo long-period complex layered structures. These structures can be described by different unit cells as 3R, 9R or 18R depending on the stacking sequences on the close-packed planes of the ordered lattice.

In the present contribution, x-ray diffraction and transmission electron microscopy studies were carried out on two copper based CuZnAl and CuAlMn alloys. X-ray diffraction profiles and electron diffraction patterns exhibit super lattice reflections inherited from parent phase due to the displacive character of the transformation. X-ray diffractograms taken in a long time interval show that diffraction angles and intensities of diffraction peaks change with the aging time at room temperature. This result reveals a new transformation in diffusive manner.

Abstract ID: 743

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Manufacturing and formation techniques

Keywords: Nanostructure, Soft materials, Lithography, Patterning, Imprinting

Nanostructures Using Soft Materials-Derived Lithography

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The main processes of engineering nanostructures are the top-down method, which is a direct engineering method for Si-type materials using photolithography or e-beam lithography. However, this direct engineering method of nano-structuring is very dependent on sensitive equipment, and have a high process cost. These are also relatively inefficient methods in terms of processing time and energy. Therefore, some researchers have studied the replication of nano-scale patterns via the soft lithographic concept, which is more efficient and requires a lower processing cost.

In this study, accurate nanostructures with various aspect ratios are created on several types of materials. A silicon (Si) nano-mold is preserved using the method described, and target nanostructures are replicated reversibly and unlimitedly to or from various hard and soft materials. The optimum method of transferring nanostructures on polymeric materials to metallic materials using electroplating technology was also described. Optimal replication and demolding processes for nanostructures with high aspect ratios, which proved the most difficult, were suggested by controlling the surface energy between the functional materials. Relevant numerical studies and analyses were also performed. Our results showed that it was possible to realize accurate nanostructures with high depth aspect ratios of up to 1:20 on lines with widths down to 50 nm.

In addition, we were able to expand the applicability of the nano-structured mold by adopting various backing materials, including a rounded substrate. The application scope was extended further by transferring the nanostructures between different types of materials with a reversible way, as well as an identical species of material.

In particular, the materials and methodologies which were suggested in this research provide the great possibility of commercially creating nanostructures as combined with an effective and reliable way. Such commercially creatable nanostructures are required for a vast range of optical parts and display devices, photonic components, physical parts and devices, energy devices, vehicles and buildings on/in the land, water or marine, and biomimetic or biosimilar structured parts and devices for antibiosis.

Abstract ID: 744

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: Thin films, band gap, IV Characteristic.

Electrical behaviour of Sm (+3) doped with CdSe FTO thin films

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Above results of Photoconductivity, optical spectra and raman studies are presented CdSe films, synthesised in aqueous solution phase at 80C by using the Chemical Bath Method. CdSe films were characterized by using different characterization. AFM, SEM and Composition studies show that films with smooth surface and well defined stoichiometry ratio of compounds. The optical values of some important parameters of the studied films were calculated by UVstudy are determined from transmission spectra at wavelength 200 to 900nm. Optical band gap Eg was calculated by tauc relation. Energy band gap of Bandgap. In Raman analysis, a prominent peak shows that confirmation of nanocrystalline phase. And intensity of peaks was decreasing after doping. From IV results shows that both dark and photo current of samples increase linearly with applied voltage.

Abstract ID: 745

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Design and application of composite structures

Keywords: Shape memory alloys, (micro)Robots, NiMn2Ga, Lattice softening, NiTi SMA.

High frequency operating shape changing resonators utilizing unique properties of SMA elements for (micro)robotics

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The magnetic field-driven (micro)robots are capable to deliver, manipulate and modify various micro-/nanoscale objects; therefore, they hold promises for either the controlled drug delivery to a specific area in human body or the non-invasive diagnosis and treatment. Currently develop magnetic field-driven robots transform the electrical energy into the mechanical work through a generated magnetic torque and/or force. However, strength of the magnetic field that drastically decreases with the distance from its source, complicates the necessary magnetic control and, consequently, restrict the widespread of these magnetic field driven (micro)robots. We report on an alternative contactless resonating architecture consisting of the polymer matrix embedded with NiMn2Ga and NiTi elements. This actuation principle utilizes the anomalous softening / hardening in NiMn2Ga caused by the magnetoelastic coupling and a low magnetic anisotropy in its austenite phase, and the intentionally changeable prestress forces generated by NiTi elements. When NiMa2Ga elements are subjected to prestress, the interplay between changes in the elastic properties of NiMn2Ga during magnetization / demagnetization and the variable prestress originating from phase transformation in NiTi enables high frequency actuation and precise control of the bending of designed structure. We develop theoretical procedure capable predicting the behavior of these vibrating structures. Due to its relevance to actuation of micro-robots, we perform detailed analysis on multiple promising swimming mechanisms. The proposed architecture paves a way for further design of micro-(bio-)robots and contactless high frequency actuators and sensors with intentionally changeable shapes.

Abstract ID: 746

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Sensors and MEMS: Materials and Devices

Keywords: Key Words: Titania nanoparticles, electron beam gun deposition, nanofabrication, gas sensor

Carbon dioxide gas sensor based on Titania nanoparticles and poly-porous silicon

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Titania Nanoparticles (TNPs) were synthesized using sol-gel and microemulsion methods with the size of 8.5 nm and 10 nm, respectively. The obtained size of nanoparticles calculated by Scherrer's formula and characterized by X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), UV-visible spectroscopy (UV-vis), and Atomic Force Microscopy (AFM). The XRD analysis explains that the prepared sample is in the pure Anatase phase with the Tetragonal crystal system. The TNPs have been deposited as a thin film on the poly-porous silicon wafer using an electron-beam gun deposition. Our sandwich device has also been prepared using electron beam gun deposition with two Aluminum electrodes on the bottom and top of the device as conductors. We exposed our nanostructured device against the different concentrations of Carbon dioxide and oxygen gas, respectively. We measured the gas sensitivity, percentages of reversibility of sensor, and response against gas using the electrical properties of our device in our lab. We conclude that the device with TNPs thin film layer is much more sensitive against gas in comparison with the device without TNPs layer. It would be a nice result that the nanofabricated device based on the poly-silicon and TNPs is a good choice to apply as a gas sensor both economically and quality to absorb gas and interact with it.

Key Words: Titania nanoparticles, electron beam gun deposition, nanofabrication, gas sensor

Abstract ID: 747

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Photonic devices and applications

Keywords: Photo-magnetism, holography, diffraction, Faraday rotation

Photo-magnetic material functioning as recording medium for dynamic computer-generated holography

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This study describes the promising marriage of novel unique photo-magnetic materials with the ultimate three-dimensional display technology, namely holography. Dynamic computer-generated holography requires extremely dense writing of interference fringes, combined with fast refresh rates and perfect transparency of the medium, allowing real-time, translucent, speckle-less display of complex wavefronts, which are truly three-dimensional and thus very natural for human vision. The capabilities of liquid crystal based devices in this matter are very far from satisfactory, although this technology has been dominant for decades. On the other hand, photo-magnetic switching of magnetic domains [1] has the potential of 60 ps switching times, theoretically allowing unprecedented GHz per-pixel modulation speeds in matrix-like configurations. We have demonstrated experimentally the feasibility of purely optical switching of magnetic domains in a photo-magnetic medium in a form of MEMS-driven point-by-point writing of holographic patterns in Cobalt-substituted yttrium iron garnet (YIG:Co) [2]. The interesting effect from the holographic standpoint is the Faraday rotation in the optically transparent sample, allowing the direct measurements of diffractive effects, tailored by the shape and density of written patterns, which are normally observed only geometrically i.e. under Faraday magneto-optical microscope. The amount of rotation in the tested samples was relatively small, but allowed a strong detection of the designed diffraction patterns in the far field behind the sample illuminated with a polarized 635 nm laser light. This study presents the unique material properties suitable for threshold-like, wavelength- and polarization-dependent operation [3] in the 1300 nm femtosecond pump beam, as well as the discussion about the potential density and uniformity of the said direct holographic recording with respect to future displays and pixel-less spatial phase-modulating devices.

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Abstract ID: 748

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanomaterials and Nanotechnology

Keywords: carbon nanotube, neural probe, CTE, TSV, interposer

Neural Probes and Through-Silicon-Via Interposers: Utilizing High Aspect Ratio Carbon Nanotube Arrays

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Assembling nanomaterials into arbitrary architectures is vital step in defining their role in any application. Vertically aligned carbon nanotubes (VACNTs) represent an interesting multifunctional nanomaterial to construct larger macroscopic assemblies for applications. In this talk, I will present our work on the fabrication and utilization of VACNT pillars. First, I will discuss our approach to enable the fabrication of high aspect ratio (60:1) free-standing CNT pillars possessing high uniformity [1-3]. To maintain perfectly vertical growth of each pillar within the array of mm-tall, high aspect ratio VACNTs, “hedge” structures were employed as support but later removed. As a result, 1.2 mm-tall and 20 um-diameter pillars were achieved. Second, I will present two diverse applications utilizing two different aspects of this porous structure. In one case, we applied these high aspect ratio and mechanically compliant posts as microelectrodes as a candidate for neural probes. Examination of the electrochemical detection to methyl viologen and dopamine using an individual CNT microelectrode showed fast-electrochemical response. In another application, we demonstrate the feasibility of CNT-Cu as a via material for through-silicon-via (TSV) interposers which can potentially possess both high electrical conductivity of Cu and low coefficient of thermal expansion (CTE) of CNTs, after a two-stage Cu electrodeposition [4, 5]. The CNT-Cu TSV showed Cu-level electrical conductivity (~2.5×10E5 S/cm) and Si-level CTE (~7×10E-6 /K). The greatly reduced CTE mismatch between CNT-Cu and Si was achieved and its functionality was demonstrated.

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Abstract ID: 749

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Carbon and metal oxide based composite materials

Keywords: Activated Carbon Nanofibers; Calcium Oxide; Nanocomposites; Adsorbents; CO2 Adsorption

Activated Carbon Nanofibers Incorporated Calcium Oxide for CO2 Adsorption

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Activated Carbon Nanofibers Incorporated Calcium Oxide for CO2 Adsorption

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In this study, activated carbon nanofibers (ACNFs) incorporated with calcium oxide (CaO) were successfully prepared via a simple electrospinning and pyrolysis process. Optimum electrospinning and pyrolysis parameters were performed to obtain porous ACNFs composites for CO2 capture. The porous and textural characteristics of the resultant ACNFs composites were performed using N2 adsorption isotherms at 77 K, while the features and morphologies were observed using TEM and FE-SEM. The EDX and Raman analysis were used to determine and analyse the elemental composition in the ACNFs. It was observed that CaO/ACNFs exhibited surface area of 236 m2/g and micropore volume of 0.13 cm3/g as compared to pristine ACNFs. CaO/ACNFs also possessed smaller fiber diameter of 663.5 ± 47.3 nm as compared to pristine one. The successful incorporation of CaO in electrospun fibers were proven by EDX analysis. All resultant ACNFs exhibited D- and G-peaks in Raman spectra indicating the carbon-based materials structure. As expected, the CaO/ACNFs attained higher CO2 adsorption of 56 cm3/g at 298 K as compared to other ACNFs samples which is correspond to N2 adsorption capacity. The CO2 adsorption/desorption isotherm of CaO/ACNFs was measured at three different temperatures (273, 298, and 318 K) at 1 bar through a volumetric adsorption process and this result was compared to ACNFs. It shown that the CO2 adsorption capacity is inversely proportional to the increasing temperature in which as the adsorption temperature increased, the adsorbed amounts of CO2 decreased. These results indicated that the incorporation of CaO into ACNFs shows improvement in their physicochemical properties for enhanced adsorption performance of CO2 under practical conditions.

Key Words: Activated Carbon Nanofibers; Calcium Oxide; Nanocomposites; Adsorbents; CO2 Adsorption

Abstract ID: 750

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Motors, Generators and Actuators

Keywords: Concentration, Transportation, NPs, Ultrasound

Controlled concentration and transportation of nanoparticles at the interface between a smooth substrate and droplet

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Controlled concentration of nanoscale materials on the surface of a smooth substrate without vibration excitation mechanism and micro channels, and transportation of the concentrated nano material on the surface, have large potential applications in the fabrication of nano sensors and electrodes, decoration and assembly of nano materials, etc. However, implementation of these two nano manipulation functions by one single device has been a big challenge. Here we report a method to concentrate nanoparticles at an arbitrary location at the interface between a smooth substrate and water droplet, and to transportation the concentrated nano material freely at the interface. It employs the acoustic streaming, which is generated by a micro manipulating probe (MMP) vibrating linearly above the substrate. SiNPs can be concentrated under the MMP at a desired location, forming a round spot of nano materials with a diameter up to 230 μm. The concentrated nano material can be transported through an arbitrary path at the interface by shifting the device, and has little change in the size and shape during the transportation. The dependency of acoustic streaming field around the MMP on device parameters is clarified by numerical computation and verified by experiments.

Abstract ID: 751

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Functionally graded composite materials and structures

Keywords: Arbitrary oriented crack, functionally graded material, heat flux intensity factor, Schmidt method, thermal loading.

Schmidt method to study a problem of heat conduction in a functionally graded layered structure with an arbitrary oriented crack

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The purpose of this article is to investigate the behavior of a partially insulated crack in a functionally graded layered structure under thermal loading. The crack is arbitrary oriented and its center is located at the interface. Employing the superposition approach and Fourier transformation, a mixed boundary value problem is reduced to a Cauchy-type singular integral equation. The unknown variable of the singular integral equation is the jump of the temperature across the crack surfaces. Representing the unknown variable as a series of Jacobi polynomials, the solution of the singular integral equation is obtained with the help of the Schmidt method. The adopted procedure is quite different from those used in the previous works, in which the unknown variables are the dislocation density functions [1-2]. With the help of the Schmidt method, the analytical form of heat flux intensity factor at the crack tips are obtained. The salient feature of the article is the pictorial presentations of heat flux intensity factors and temperature fields in the vicinity of the crack tips. A drive has been taken to quantify the effect of partial insulation of the crack surfaces, crack orientation, layers' thickness, and material non-homogeneity parameters graphically.

Abstract ID: 752

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: Cadmium sulfate, L-Valine, Birefringence, AIM, dielectric susceptibility, DTA-DSC, Gibbs and chemi-potential

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The metal sulfate compound blended with organic base; L-Valine and respective crystal was synthesized. The XRD peaks with moderate intensity at corresponding planes showed orthorhombic crystal lattice. The unit cell parameters; a=5.811 (Å), b=8.932 (Å) and c=6.963 (Å) and associated indices of refraction was n1=1.611, n2=1.533 and n3=1.789. The birefringence region; 0.078-0.256 explicit NLO efficiency 3.298 I2□= X I2□. The mulliken charge distortion analysis made and its chemi-equipotential nodal region in molecular site was mapped. The kinetic energy distribution over molecular structure and electron density critical point data was acquired from AIM results and summing of chemical potential was identified. The restored chemical potential for the application of NLO and birefringence was checked by opting crystal controlled parameters. The scattering capability of homo nuclear and hetero nuclear bonds was measured and linear scattering process was notified in observed IR and Raman lines. The blown interactive orbitals for degenerate energy levels of different molecular segments were sketched using energy distribution grid points and associated chemical potential exchange among important molecular zones were studied. The EDAX data was obtained for measuring stoichiometric ratio of elemental parts of the crystal. The dielectric multipole moments were estimated and thereby dielectric susceptibility was determined in different coordinates of the molecule. The thermal breaking point and hardness along with Gibbs energy continuity was located and the rigidity was measured.

Abstract ID: 753

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: neurotransistor, silicon nanowires, field effect transistor

Silicon nanowires based artificial neuron

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Learning processes similar to those occurring in a human brain can also be realized relying on brain-inspired computers. To implement a device like a biological neuron, it is necessary to trigger chemical processes occurring in a neuron cell directly within the electronic device. For example, the device should be able to transfer ions or molecules and store their instantaneous distributions as ‘states’, which should be subsequently controlled in response to external stimuli. Here we report a neurotransistor made from a silicon nanowire transistor coated by an ion-doped sol–gel silicate film that can emulate the intrinsic plasticity of the neuronal membrane. The neurotransistors are manufactured using a conventional complementary metal–oxide–semiconductor process on an 8-inch (200 mm) silicon-on-insulator wafer. Mobile ions allow the film to act as a pseudo-gate that generates memory and allows the neurotransistor to display plasticity. We show that multiple pulsed input signals of the neurotransistor are non-linearly processed by sigmoidal transformation into the output current, which resembles the functioning of a neuronal membrane. The output response is governed by the input signal history, which is stored as ionic states within the silicate film, and thereby provides the neurotransistor with learning capabilities.

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Abstract ID: 754

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Hybrid cells for energy harvesting

Keywords: Monolayers, Organic Semiconductors, Perovskite Solar Cells

Self-Assembling Monolayers - Effective Approach for Efficient Perovskite Solar Cells

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Perovskite-based photovoltaics promise benefits of low cost, high efficiency and large versatility. However, combining all three factors into one solar cell is a difficult task. In particular, one of the bottlenecks towards large-scale production is the available choice of hole-selective contacts. Self-assembled monolayers as hole-selective contacts are a viable alternative to classic hole transporting materials as they are intrinsically scalable, simple to process, dopant-free and inexpensive. Self-assembly also offers the crucial advantage of conformally covering rough surfaces within a self-limiting, simple to control process, creating energetically well-aligned interface to the perovskite absorber with minimal non-radiative recombination. This approach enables highly efficient single-junction p-i-n perovskite solar cells and record-efficiency monolithic perovskite/CIGSe (24.2%) as well as perovskite/silicon (PCE up to 29.15%) tandem devices.

Abstract ID: 755

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Electrode/electrolyte interface phenomena

Keywords: Nitrate, membrane reactor, electrocatalysis, kinetics

Role of Copper nano particles in attaining electrocatalytic reduction reactions

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The electrocatalytic reduction of NO3- and its intermediate NO2- in neutral medium was performed at Cu- Nano particles immobilized Pt surface. The voltammetric investigations showed that bare Cu electrode has a little effect on nitrate reduction reactions (NRR). Whereas, an enhanced catalytic effect (i.e. a positive shift of the peak potential and an increased reduction current) was obtained when Cu NPs were immobilized onto the Pt surface. The NRR process occurred via a two-step mechanism at the Pt-Cu surface with the transfer of 2 and 6 electrons, respectively. The results were further validated by chronoamperometry (CA) investigations. In the present work conditions, the NRR proceeded via a simple adsorption-desorption mechanism following a Langmuir isotherm with an adsorption Gibbs free energy of ca. −10.16 KJ.mol−1 (1st step) and ca. -10.05 KJ.mol-1 (2nd step). By means of a Pt│Nafion│Pt-Cu type reactor without any supporting electrolyte, bulk electrolysis was performed to identify the step products. It was found that after 180 min long electrolysis, 51% of NO3- was noticed to convert into intermediate NO2-. This percentage decreased to 30% in CO2 buffered condition. However, when a tri-metallic Pt-Pd-Cu was employed as a cathode, all of the evolved NO2- could successfully be converted into NH3 and N2. In contrast to reported works concerning Cu electrodes, the as prepared Pt–Cu catalyst in this study showed no apparent surface poisoning as confirmed by its stability after excessive CV runs as well as successively extended electrolysis.

Abstract ID: 756

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Industrial applications of composite materials

Keywords: Clay composites, arsenic and p-nitrophenol removal, landfill leachate treatment

Innovative composite sorbents for organic and inorganic pollutants removal from aqueous solutions in landfill leachates

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The study reveals the development of appropriate innovative sorbents based on clay material for arsenic and p-nitrophenol sorption using iron oxy-hydroxide and surfactant modification. Natural and manufactured clay were chosen for comparison of modification efficiency to obtain the best sorption results for As (V) and p-nitrophenol. Obtained results indicate that modification of clay with iron compounds and various surfactants significantly improve the sorption capacity of newly developed materials used for sorption of inorganic and organic compounds from aqueous solutions in landfill leachates.

Natural clay minerals have received a lot of attention as potential sorbents, because of their abundance, cheapness, high sorption and ion-exchange properties [1]. Clay minerals can be modified using different approaches to obtain innovative materials for application as sorbents in the removal of inorganic and organic pollutants from leachates, wastewater, groundwater and soil [2, 3]. Modification with surfactants improves hydrophobization needed if interaction with low polarity organic molecules is necessary, but chemical modification with inorganic species, e.g., hydrated iron supports the physical improvement of sorption and ion exchange process in order to benefit the treatment of media from inorganic pollutants [4]. Materials achieved better properties for specific remedial applications regarding heavy metals and metalloids, prepared organoclays from hydrophilic montmorillonite by intercalating cationic or nonionic surfactants can interact with organic molecules of differing polarity and serve as immobilizers for organic molecules and toxicants, e.g., phenols and NOCs. Further studies will reveal improved properties to benefit landfill leachate treatment, wastewater engineering and environmental remediation industries. The research was supported by project No.1.1.1.2/VIAA/3/19/531 “Innovative technologies for stabilization of landfills—diminishing of environmental impact and resources potential in frames of circular economy”.

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Abstract ID: 757

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Photonic devices and applications

Keywords: aqueous dye extract, Zinc oxide, optical properties

Influence of aqueous dye extract and annealing treatments on the optical properties of chemically deposited Zinc Oxide thin films for Use in Optoelectronic Devices

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The study reports on the influence of aqueous dye extract and post-deposition heat treatments on the optical properties of Zinc oxide (ZnO) thin films prepared by a simple low cost chemical bath deposition technique. The results indicate that the optical properties of the films were modified significantly by the processing conditions. The transmittance of the dye-coated films was generally lower compared to that of the as-grown films. The optical constants of the coated films varied in one direction while that of the as-grown films varied in the reverse direction. The energy bandgap of the coated films where typically higher than that of the as-grown films. The annealing treatments decreased the energy bandgap for aqueous dye coated films annealed between 100 oC to 300 oC, and increased the energy bandgap in the as-grown films annealed under similar post deposition heat treatments. The values of the optical constants strongly indicate that the films will be useful in different optoelectronic applications including sensing devices. This study reveals that aqueous dye extract can be used to tailor the properties of ZnO thin films for enhanced application in different solar architecture and optoelectronic devices.

Abstract ID: 758

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Processing and manufacturing technologies

Keywords: water jet cutting, lignin-based polymers, roughness

Water Jet Cutting influence on lignin-based polymers parts

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Arboblend V2 Nature and Arbofill Fichte combine a series of characteristics focus directly with its chemical composition. The materials have a high level of biodegradability and as constituent's can be counted biopolymers such as lignin, polylactic acid (PLA), starch, natural resins and waxes, etc. So far, in the technical literature, there are no experimental results on this lignin-based materials on machinability by water jet cutting, a technological process very often used in industrial practice. Thus, the article aims to establish experimentally and theoretically the solutions for optimizing the working regime for processing with water jet with abrasive in order to obtain a higher quality surface compared with the currently existing ones for biodegradable polymeric materials. The main aspects of water jet abrasive processing are surface roughness, hardness and dimensional accuracy. Also, the article performs an experimental analysis on the technological parameters effects regarding the quality surface and dimensional accuracy of the parts. The main technological parameters of the process taken into account were as follows: cutting quality level, feed rate and distance between the processing head and the cutting part.

Abstract ID: 759

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Porous and cellular materials

Keywords: Macroporous cryogel, Oxidation of aliphatic alcohols, Flow-through catalytic reactor

Flow-through catalytic reactor based on macroporous polyampholyte cryogels for oxidation of aliphatic alcohols

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Aliphatic alcohols (ethanol, n-propanol, iso-propanol, n-butanol, iso-butanol) were oxidized by catalase encapsulated within strong charged polyampholyte cryogels derived from anionic monomer – 2-acrylamido-2-methyl-1-propanesulfonic acid sodium salt (AMPS) and cationic monomer – (3-acrylamidopropyl) trimethylammonium chloride (APTAC). Macroporous polyampholyte cryogels containing various amounts of catalase was synthesized in situ cryo-polymerization conditions at molar ratio of monomers [APTAC]:[AMPS] = 75:25 mol/mol in presence of 10 mol.% crosslinking agent – N,N-methylenebisacrylamide (MBAA). Catalytic oxidation of aliphatic alcohols was carried out in aqueous solution in model flow-through catalytic reactor at a flow-rate of the mixture of substrate and hydrogen peroxide 3-6 mL□min-1. Chromatographic and chromatomass spectroscopic analysis shows that aliphatic alcohols are converted to corresponding aldehydes and ketones with 85-99% yields at room temperature and atmospheric pressure. SEM images of cryogel-encapsulated catalase before and after several cyclic oxidation reaction show the complete difference in cryogel morphology due to changing of the morphology of cryogel matrix. Based on commonly accepted approaches, the oxidation mechanism of aliphatic alcohols by cryogel-encapsulated catalase is suggested.

Abstract ID: 760

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanomaterials and Nanotechnology

Keywords: Coprecipitation, Nanoparticles, Surfactant, FESEM, Photocatalytic

Effect of CTAB surfactant concentration on CdO nanoparticles in Photocatalytic applications

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Effect of CTAB surfactant concentration on CdO nanoparticles in Photocatalytic applications

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Abstract

Cetyl Trimethylammonium Bromide (CTAB) assisted cadmium oxide (CdO) nanoparticles have been synthesized with varying concentration of CTAB surfactant (0.00M, 0.04M, 0.08M, 0.12M) by using co-precipitation technique. Properties of pure CdO nanoparticles have been compared with that of CTAB assisted CdO nanoparticles. Structural properties and surface morphology have been studied with the aid of X-ray diffraction (XRD) and Field Emission Scanning Electron Microscope (FESEM) respectively. Presence of elemental compositions is also confirmed by Elemental Dispersive X-ray Spectroscopy (EDS). Raman spectroscopic evaluation is also done to study the modes of vibrations created due to change in concentration of CTAB. Fourier transform infrared (FTIR) spectra is studied to find out various types of chemical bonding present in the material. Effect of various concentration of CTAB on optical band gap of CdO nanoparticles is also studied with the help of UV-Visible spectroscopy. In photocatalytic application, degradation of Methylene Blue (MB) dye by Ultra Violet (UV) light source with distinct concentration of CTAB in CTAB assisted CdO nanoparticles is studied.

Key Words: Coprecipitation, Nano, Photocatalytic

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Abstract ID: 761

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster/Oral Presentation

Topics: Optical properties and spectroscopy of graphene and other two-dimensional materials

Keywords: Quantum Spin Hall effect, Type II Weyl semimetal, Electron-phonon coupling, Raman spectroscopy

Tailoring the Phase Transition and Electron-Phonon Coupling in 1T′-MoTe2 by Charge Doping: A Raman Study

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The transition metal dichalcogenides (TMDs) display a wide spectrum of important phenomena which give rise to various potential applications as well as rich physics. While the semiconducting 2H phase shows promising nano-electronic and optoelectronic applications, the 1T′ phase of TMDs has also recently drawn a lot of interest because of its predicted quantum spin Hall (QSH) behavior. In addition to the QSH phase at room temperature [1], 1T′-MoTe2 also undergoes an inversion symmetry breaking to give rise to a Type II Weyl semimetal (Td phase) at ~250 K [2]. While it is very exciting to observe two important topological phases in a layered 2D material, it has been reported that the phase transition gets suppressed for thin flakes of MoTe2 [3,4]. In our work, we have demonstrated an important pathway for switching between the two topological phases of MoTe2 by means of charge doping [4]. Hole doping and electron doping were observed to stabilize the 1T′ and Td phases, respectively [4]. On the other hand, MoTe2, being a low Tc superconductor, also displays strong electron-phonon coupling. Our Raman-based measurements reveal a charge doping-dependent electron-phonon coupling in MoTe2 [4]. We, therefore, demonstrate the possibility of simultaneously tuning the two very important phenomena of topological phase transition and the electron-phonon coupling in MoTe2 by charge doping. This further establishes a connection between the electron-phonon coupling and topological phase transitions, which might be of vital importance in the understanding of the underlying physics in quantum phenomena observed in TMDs and related potential applications.

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Abstract ID: 762

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Electrochemical Supercapacitors

Keywords: Supercapacitors, negative electrode materials, graphene, spinel oxide

Negative Electrode Materials for Supercapacitive Energy Storage: Bottlenecks and Possible Remedies

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Although benefiting from the intrinsic advantages of high-power capability and long cycling stability, the low energy performance has limited, to some extent, broader feasible applications of supercapacitors.1 Energy of a supercapacitor can be increased by either increasing the device capacitance or extending the operating voltage window. Compared with the positive electrode materials that have made incredible progress thus far, the lack of high capacitance negative electrode materials is still a bottleneck for making further progress toward high device-level capacitance supercapacitors. As a remedy to this challenge, we have pursued some high-capacitance negative electrode materials via grafting organic redox active species onto carbon-based materials.2,3 In one approach, we conjugated thionine and Nile Blue as redox active aromatic dyes to graphene aerogel via π-π stacking interactions. Via this simple yet effective approach, we obtained highly stable negative electrode materials with enormously higher supercapacitive performances. In another approach, we prepared a CoFe2O4-rGO nanocomposite via a scalable one-pot solvothermal method that delivers high capacitance as a negative electrode material.4 Via these intriguing approaches we have fabricated some high-energy supercapacitor devices without sacrificing their intrinsic high-power capability and long cycling stability.

Abstract ID: 763

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Solar Cells

Keywords: Open-circuit voltage, Thermodynamics, Energy conversion materials

Thermodynamic interpretation of the open-circuit voltage in energy conversion materials

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Renewable energy converter, such as solar energy converter or thermoelectric converter, are inherently nonequilibrium systems. For example, the driving force in solar energy converter is given by the illumination. The performance of solar cell operation can be assessed by the efficiency that relates the useful output power to the total power incident. The useful output can be interpreted as the work against an applied load and the current-voltage characteristic of a solar cell represents all possible working points as function of the voltage (applied load). The discussion of fundamental limits to photovoltaic efficiencies, the enhancement of power conversion efficiencies, and efficiency forecasts has been guided the research activities in the field of renewable energy conversion. Efficiency limits can be obtained by thermodynamic arguments, for example, when looking at the zero-power operation of a solar cell or when looking at the maximum power point. The zero-power limit of a solar cell is given either under short-circuit operation, Jsc(V=0), or under open-circuit operation. The open-circuit voltage defines a stopping point Voc at which the applied voltage stops the current, i.e., J(Voc)=0. Focusing on state models for bulk heterojunction organic solar cell that includes the essential optical and interfacial electronic processes, we show that the open-circuit voltage is a special thermodynamic equilibrium point, at which the state occupation probability is given by Gibbs-like distribution. The Gibbs-like distribution which can be used to calculate both the entropy of the stopping configuration and the entropy of the equilibrium reference state. An interesting quantitative measure of the difference between the stopping configuration and its associated “true” equilibrium configuration is given by the so-called relative entropy or Kullback-Leibler entropy (divergence). The Thermodynamic interpretation of the open-circuit voltage provides a framework to calculate analytically the open circuit-voltage in dependence on the underlying microscopic processes. This study offers a promising route to include different types carrier recombination processes and discuss its consequence on the open-cuircuit voltage.

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Abstract ID: 764

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Silver Nanoparticles, Des-γ-Carboxy Prothrombin, Carbon Tetrachloride, Hepatotoxicity.

Assessment Study of Des-γ-Carboxy Prothrombin Level After Treatment with silver nanoparticles in Male Rat Induced by Carbon Tetra-Chloride

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The present study was conducted on 110 males of Wistar rat weightings (190-300 g), aged (15-17) weeks, at the animal house faculty of science/university of Kufa during the period from December 2019 to July 2020. This study included assessed des-gamma carboxyprothrombin level of evaluating the protective role of the phenolic extract of Urtica dioica leaves (250 and 500 mg/kg) against hepatotoxicity induced by carbon tetrachloride. The animals experimental are divided into 22 groups (n= 5 rats per each group) for the duration of two and three months. The levels of biomarker proteins (Des-gamma carboxyprothrombin), were measured in control groups, carbon tetrachloride groups, and the phenolic extract of Urtica dioica groups. The results showed a significant increase ($P \leq 0.05$) in serum levels of biomarker proteins (Des gamma carboxy prothrombin) in carbon tetrachloride groups as compared with the control group. Biomarker proteins (Des gamma carboxy prothrombin) in groups treated with phenolic extract of Urtica dioica as compared with carbon tetrachloride group. The present study concluded that both phenolic extracts of Urtica dioica leave had a protective effect on hepatotoxicity in the carbon tetrachloride-induced group.

Abstract ID: 765

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Strontium ferrate, Perovskite, Mechanosynthesis, Mössbauer spectroscopy, XPS

Structural and magnetic studies of mechanosynthesized Nd-doped SrFeO3−d Nanocrystalline particles

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We report on the mecahosynthesis, structural and magnetic characterization of 10 at% Nd-doped perovskite-related SrFeO3-δ nanocrystalline particles (~80 nm) using XRD, Mössbauer spectroscopy and vibrating sample magnetometry (VSM). The material is formed starting from a 120h pre-milled stoichiometric mixture of a-Fe2O3, Nd2O3 and SrCO3 at 800 oC which is ca. ~ 300oC lower than those at which cation-doped SrFeO3-δ bulk modifications are conventionally prepared. Rietveld refinement of the XRD data and 57Fe Mössbauer spectra have revealed these Fe4+/Fe3+ mixed-valence nanocrystalline particles to be composed of cubic Nd0.1Sr0.9FeO3 and oxygen-deficient tetragonal Nd0.1Sr0.9FeO2.875 phases in the ratio of ~ 45 : 55. The Mössbauer results also show the Nd-doped SrFeO3-δ nanoparticles to be superparamagnetic with blocking temperatures below 78K. A complex magnetic behavior, associated with the coexistence of the cubic and tetragonal phases, is detected for the nanoparticles wherein an antiferromagnetic-to-paramagnetic transition and an antiferromagnetic-to-weak ferromagnetic transition were detected at ~ 61 K and ~24 K, respectively. XPS measurements reveal a complex surface structure of the Nd-doped SrFeO3-δ nanoparticles where traces of the initial reactants, viz. a-Fe2O3 and SrCO3, were detected.

Abstract ID: 766

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Electrical, optical, electrochemical, thermal and mechanical properties of graphene, Mxenes and other two-dimensional materials

Keywords: graphene, van der waals force, 2D materials

Solid-State Lifshitz-van der Waals Repulsion through 2D Materials

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The van der Waals 1 (vdW) force is a ubiquitous short-range interaction between atoms and molecules that underlies many fundamental phenomena. Early pairwise additive theories pioneered by Keesom, Debye, and London suggested the force to be monotonically attractive for separations larger than the vdW contact distance. However, seminal work by Lifshitz et al. predicted that quantum fluctuations can change the sign of vdW interactions from attractive to repulsive. Although recent experiments carried out in fluid environment have demonstrated the long-range counterpart – the Casimir repulsion, it remains controversial whether the vdW repulsion exists, or is sufficiently strong to alter solid-state properties. Here we show that the atomic thickness and birefringent nature of two-dimensional (2D) materials, arising from their anisotropic dielectric responses, make them a versatile medium to tailor the many-body Lifshitz-vdW interactions at solid-state interfaces. Based on our theoretical prediction, we experimentally examine two heterointerface systems in which the vdW repulsion becomes comparable to the two-body attraction. We demonstrate that the in-plane movement of gold atoms on a sheet of freestanding graphene becomes nearly frictionless at room temperature. Repulsion between molecular solid and gold across graphene results in a new polymorph with enlarged out-of-plane lattice spacings. The possibility of creating repulsive energy barriers in nanoscale proximity to an uncharged solid surface offers technological opportunities such as single molecule actuation and atomic assembly.

Abstract ID: 767

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Photonic devices and applications

Keywords: Light-emitting diodes, quantum dots, superlattices

Two-Dimensional Nanoplatelet Superlattices Overcoming Light Outcoupling Efficiency Limit in Quantum Dot Light-Emitting Diodes

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Quantum dot (QD) light-emitting diodes (LEDs) are emerging as one of the most promising candidates for next-generation displays. However, their intrinsic light outcoupling efficiency remains considerably lower than the organic counterparts, because it is not yet possible to control the transition-dipole-moment (TDM) orientation in QD solids at device level. Here, using the colloidal lead halide perovskite nanoplatelets (NPLs) as a model system, we report a directed self-assembly approach to form two-dimensional superlattices (2DSLs) in which the out-of-plane vector is perpendicular to the substrate plane. The ligand and substrate engineering yields close-packed planar arrays with the side faces linked to each other. Emission polarization in individual NPLs rescales the radiation from horizontal and vertical transition dipoles, effectively resulting in preferentially horizontal TDM orientation. Based on the emissive thin films comprised of stacks of 2D superlattices, we demonstrate an enhanced ratio of horizontal dipole as revealed by 2D k-space spectroscopy. Our optimized single-junction QD LEDs showed peak external quantum efficiency of up to 24% and current efficiency exceeding 100 cd A-1.

Abstract ID: 768

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Graphene, Mxenes and other two-dimensional materials for biomedical and healthcare applications

Keywords: Nanocarbons, 3D Graphene, Bioelectronics, Neurons, Cardiomyocytes, Electrophysiology

Forming input/output (I/O) interfaces with excitable cells and tissue using nanocarbons

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We focus on developing a new class of nanoscale materials and novel strategies for the investigation of biological entities at multiple length scales, from the molecular level to complex cellular networks. Our highly flexible bottom-up nanomaterials synthesis capabilities allow us to form unique hybrid-nanomaterials that can be used in various input/output bioelectrical interfaces. For example, we have developed several bioelectrical platforms based on graphene, a two-dimensional (2D) atomically thin carbon allotrope. We have demonstrated recording of the electrical activity of excitable cells with graphene-based ultra-microelectrodes as small as the size as an axon ca. 2μm in size. Using graphene-based hybrid-nanomaterials, we have formed remote, non-genetic bioelectrical interfaces with excitable cells and modulated cellular and network activity with high precision and low needed power. We have also developed a breakthrough bioelectrical interface, a 3D self-rolled biosensor arrays (3D-SR-BAs) of either active field effect transistors or passive microelectrodes to measure both cardiac and neural spheroids electrophysiology in 3D. Our approach enables electrophysiological investigation and monitoring of the complex signal transduction in 3D cellular assemblies toward an organ-on-an-electronic-chip (organ-on-e-chip) platform for tissue maturation investigations and development of drugs for disease treatment. In summary, the exceptional synthetic control and flexible assembly of nanomaterials provide powerful tools for fundamental studies and applications in life science and open up the potential to seamlessly merge either nanomaterials-based platforms or unique nanosensor geometries and topologies with cells, fusing nonliving and living systems together.

Abstract ID: 769

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Solar Cells

Keywords: Poly(3-hexylthiophene), regioregularity, organic solar cell.

Engineering of regioregularity and energy levels of donor material for organic solar cell application.

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Climate action is a 13th sustainable development goal (SDG) of United nation that keeps renewable energy is a topmost priority of policy makers. The search of renewable energy sources is the important target of today's world. Solar energy is one of the great sources of energy. Solar cells have been developed and intensively are being used. But there is some architecture, economic and environmental limitation for use of Silicon solar cell. But most of these limitations can be avoided by the use of organic solar cell. A flexible, transparent, low cost fast printing processing, and more adoptable in modern world are some key advantages of Organic solar cell. There is also big capacity of improvement in organic solar cell regarding efficiency, environment and cost-effectiveness greener production etc. that can overcome by study of active materials. The major component of organic solar cell is acceptor material such as Fullerene and donor material such as Poly(3-hexylthiophene), P3HT. Fullerene is an ideal material but engineering of P3HT is required to enhance the efficiency of the devices. Optoelectronic properties of P3HT can be enhanced by controlling the regioregularity, Energy band gap and molar mass of polymer. The optimal conditions synthesis of efficient P3HT were studied. For commercialization of Organic solar cell, the cost effective and stereoselective method is proposed for the development of Regio-regular P3HT, that is oxidative coupling of 3-hexylthiophene (monomer) by anhydrous FeCl3 under applied external electric field, which is a novel method. Energy band gap of Synthesized polymer was also compressed by voltammetric p-doping. This research is the collection of knowledges for the engineering of efficient materials for organic solar cell.

Abstract ID: 770

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster/Oral Presentation

Topics: Mechanical and Thermal properties of graphene, Mxenes and other two-dimensional materials

Keywords: Raman spectroscopy, interfacial thermal conductance per unit area, thermal conductivity

Enhancement of Interfacial Thermal Conductance in Hexagonal Boron Nitride (h-BN)-Graphene Heterostructures

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Monolayer graphene shows excellent electronic properties thus making it a potential candidate for nanoscale device-based technology. However, to improve the device performance, better heat management of such nanoscale devices is very important. It has been reported that hexagonal boron nitride (h-BN) supported graphene, enhances (opto)electronic and thermal properties as compared to SiO2/Si supported graphene. To understand the substrate effect on heat dissipation, we have performed temperature and power dependent Raman Spectroscopic measurements on four different types of (hetero)structures: (a) h-BN (BN), (b) Graphene (Gr), (c) h-BN on Graphene (BG), and (d) graphene encapsulated by h-BN layers from both top and bottom (BGB), all supported on SiO2/Si substrate. We find that there is an improvement in both thermal conductivity and interfacial thermal conductance per unit area in the BGB heterostructures, which ensures a better heat dissipation in devices. The κ and g of h-BN encapsulated graphene on SiO2/Si (BGB) sample was observed to be 850.0 ± 81.0 W m-1 K-1 and 105 ± 1 MW m-2 K-1, respectively, as opposed to 600.0 ±93.0 W m-1 K-1 and 1.15±0.40 MW m-2 K-1, respectively, for graphene on SiO2/Si substrate. Therefore, we propose that graphene-encapsulation with h-BN from top and bottom is a suitable one to address heat management issues in graphene-based nanoscale devices.

Key Words: Raman spectroscopy, interfacial thermal conductance per unit area, thermal conductivity

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Abstract ID: 771
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Smart Composites
Keywords: Stretchable Electronics, Dielectric Elastomer, Single-Walled Carbon Nanotube, Interpenetrating Network

Making stretchy dielectric, conductive, and semiconductor polymers

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The increasing demand for devices that are deformable, wearable, or implantable has been driving the development of functional materials that are additionally compliant and repeatedly stretchable. I will introduce our recent efforts in developing elastomeric dielectrics, semiconductors, and conductors. The formation of interpenetrating networks and other microstructural control techniques are used to (1) enhance the electromehcanical responses of dielectric elastomers, (2) protect the conductive percolation network of silver nanowires and carbon nanotubes at large-strain deformations, and (3) to impart elastic deformability to semiconductor materials that are otherwise not stretchy. Explorations of devices incorporating these materials will also be presented.

Abstract ID: 772

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multi-scale Modeling of Graphene- and Carbon Nanotube-Reinforced Composites

Keywords: Graphene, Nanocomposite, Fracture

Simulation of Fracture in Graphene-Polymer Nanocomposites using Molecular Dynamics

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There is now significant experimental evidence that the dispersion of a few weight percent of nanoscale particles in a polymer matrix helps to mitigate its brittleness and microcracking without incurring serious weight penalty, thereby enhancing its fracture toughness. In addition, there is further experimental evidence that particle size plays an important role in toughness enhancement. Fracture at the nanoscale is very different from the macroscale due to nonlocal effects and non-bonded interactions. Consequently, in this paper, molecular dynamics (MD) is employed to simulate the fracture process in a polymer in the presence of dispersed nanographene platelets. In the MD study presented in this paper, a 14 nm long graphene nanoparticle (GNP) is embedded in a block of thermosetting polymer EPON 862 and curing agent DETDA, having dimensions of 30.5 nm ×31 nm ×3.4nm, with an edged crack of length 13.5nm as shown in Fig. 1. This was model was developed to determine the improvement of fracture properties using the atomistic J integral as a suitable metric for evaluation of toughness at the nanoscale. After densification of the system at 300K using the NPT ensemble with a pressure of 0.1 atm, the system temperature was increased in a stepwise manner from 300K to 500K using Noose-Hoover thermostat for 10 ps to enable crosslinking of the epoxy utilizing the ReaxFF force field. This resulted in a model with 80% crosslinking density and a bulk density of ~1.2 g/cm3. The GNP was then annealed intrinsically within the polymer block to 300K. The annealing of the polymer with embedded GNP results in slight wrinkling of the GNP, as shown in Fig 1, analogous to what is observed in experiments. The system was then subjected to uniaxial isothermal straining in the y-direction to determine its fracture properties. Also, three concentric contours around the crack was utilized to investigate the path independence of the computed J-integral. Additional MD simulations are planned where two 7 nm long GNP platelets are embedded in the polymer block replacing the single 14 nm platelet, in order to study the effect of platelet length on toughness while keeping the GNP weight percentage constant. Results pertaining to fracture toughness properties for both cases will be presented.

Abstract ID: 773

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrode/electrolyte interface phenomena

Keywords: Lithium Metal Batteries, Energy Storage, Dendrite, Solid-State Electrolytes, Molecular Dynamics

Dendrite Growth Mechanism in Solid-State Electrolytes of Lithium Metal Batteries by Molecular Dynamics

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Lithium metal batteries are gaining increasing attention in the field of electric vehicles due to their high theoretical capacity and low electrochemical potential. However, unique drawbacks, including uncontrolled lithium dendrite growth, high chemical activity, and large volume changes, prevent large applications of stable Li metal anodes. Therefore, solid-state electrolytes (SSE) are recently proposed to be the ultimate remedy to solve the dendrite growth issues for the development of high-energy-density and highly safe batteries. Unfortunately, contrary to the general understanding, things didn't work the way researchers predicted. Recent reports have indicated that Li dendrites form easily in the practical SSE systems at the poor interfaces or along large grain boundaries of the SSE. But, the facile characterization techniques to track the detailed and in-depth interfacial evolution information on SSEs are currently lacking. Therefore, in this study, the authors try to comprehensively investigate the mechanism of dendrites growth in solid-state electrolytes by using molecular dynamics. These efforts will help in the rational design of dendrite-free Li metal batteries, to open a new chapter in future energy storage systems.

Abstract ID: 774
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Bio-inspired design of composites
Keywords: Bionanocomposite, Chitosan, Green Synthesis

Benign Green Synthetic Routes of Functional Chitosan-Metal Nanocomposite Bioinorganic Materials

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Fundamentally, green synthesis is a sustainable method that is benign by design. The process reduces or eliminates the use or generation of harmful substance to the environment. Green synthesis of chitosan-metal bionanocomposites involve three main steps which are evaluated based on green chemistry perspectives [1]. The first component is selection of solvent medium that is environmentally friendly. Second is the choice of reducing agent or method employed for the metal nanoparticles and the last is based on the use of nontoxic stabilizing agents. Typically, couple of green chemical methods have been employed in our group to produce different functional bionanocomposites with biopolymeric chitosan as the main sustaining stabilizing agent. The protocol is premised on the ability of chitosan to effectively co-ordinate selective metal ions via electron rich amino groups on the polymer chain before reduction which further takes place along with oxidation of the hydroxyl groups. Details of these green routes as well as functional abilities of the resultant open-network with high surface area bionanomaterial in several fields of environmentally sustainable practices will be presented

Abstract ID: 775

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Nanomaterials and Nanotechnology

Keywords: targeted nanoparticles, type 1 diabetes, immunoregulation, drug delivery

Preclinical Efficacy of MECA79-anti-CD3-Nanoparticles in Reversing Type 1 Diabetes

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Nanoparticles (NPs) have emerged as highly innovative materials to targeted delivery. Targeted drug carriers using polymeric-NPs hold particular promise to enhance the delivery of immunoregulatory agents to treat Type 1 Diabetes (T1D). We have recently formulated anti-CD3 loaded MECA-NP (MECA79-anti-CD3-NP) and showed their utility in prolonging heart allograft survival. We showed a significant increase in the T reg population in the draining lymph node (DLN) of MECA79-anti-CD3-NP treated transplanted animals and increased delivery to the DLN. We also fully characterized the fragments of MECA79 mAb following the reduction assay using TCEP, which shows mostly monomeric antibody. The average diameter of NPs was determined using dynamic light scattering to be 80.9±2.88 nm and 123.7±8.3 nm prior to MECA79 mAb conjugation and post-conjugation, respectively ($p<0.01$, n=3/group). To validate controlled release of anti-CD3 Ab from NPs, we studied the release profile of anti-CD3 up to two weeks in vitro. The results confirmed the gradual release profile of the anti-CD3 over time. Use of organic solvents during the NP fabrication step may affect the function of the antibodies. We then tested the preclinical efficacy of MECA79-anti-CD3-NP in reversing hyperglycemia in NOD mice (n=9 mice). Treatment was started at second consecutive day of blood glucose >250 mg/dL with i.v. administration of MECA79-anti-CD3-NP for five consecutive days followed by once a week treatment for 3 more weeks (n=7) (5 µg of anti-CD3/day/mouse). Amongst the 9 treated mice with MECA79-anti-CD3-NP, 7 mice responded to the treatment within a week (~78% acute remission rate) vs. 37% for the free anti-CD3 group (3 out of 8 mice). Free disease rate at day 45 (long-term remission rate was 75% for the MECA79-anti-CD3-NP and 40% for free anti-CD3 group. NO remission was noted in the untreated group (Figure 1). These data show a significant increase in therapeutic efficacy of anti-CD3 when it is delivered in the format of MECA79-anti-CD3-NP. It should be noted that these data for the first time showing the targeted delivery and superior efficacy using targeted nanoparticles in T1D. We sacrificed 2 normoglycemic NOD mice treated with MECA79-anti-CD3-NP. In contrast to the hyperglycemic NOD with no viable islets, there were viable insulin stained islets with T cell infiltrates around the islets (Figure 2).

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Abstract ID: 777
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Processing and manufacturing technologies
Keywords: additive manufacturing, lignin, material characterization

Additive manufacturing of bio-based polymers

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During the last years, there has been an increased interest in the use of 3D Printing technologies in many industrial applications and it have been identified as one of the most promising production technologies. Besides the modern equipment of 3D printing and the possibilities of industrial use of the different benchmarks the paper presents also some experimental results for "liquid wood" parts by 3D printing and compared to other biodegradable materials such as PLA, HD PLA, Impact PLA, Biofila, Fiber Wood, Extrudr BDP Flax, Extrudr BDP Pearl etc. The results will focus on mechanical properties including micro and nano indentation tests, tribological properties, Dynamic Mechanical Analysis, tribological behaviour, thermal and micro structural analysis. Take into account the results with different plastics can be concluded that the used biodegradable materials have superior quality and strength that meet the technological demands, replacing successfully the market giant-plastic within all activity fields.

Abstract ID: 778
Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)
Invited Talk
Topics: Superconductivity and Superfluidity
Keywords: Magnetic Levitation, Superconductors, MAGLEV transportation

CAN MAGLEV TRANSPORTATION BECOME ONE OF THE MAIN APPICATIONS OF SUPERCONDUCTORS ?

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Magnetically levitated (MAGLEV) transportation systems are more and more considered as alternatives to classical railways. In this contribution, we'll detail the different technologies [Electro-Magnetic Levitation (EML), Electro-Dynamic Levitation (EDL) and Superconducting Magnetic Levitation (SML)] explored and the present realizations emphasizing their advantages and disadvantages. Then, we'll focus on Superconducting Magnetic Levitation. We'll detail the properties of the magnetic field sources and of the superconductors employed and the magnet–superconductor interaction. We'll describe the main numerical simulation techniques and analytical calculations used to reproduce the behavior of levitating systems. Finally, we'll report recent results obtained by our group on the conditions of stability of levitating systems and for increasing their levitation force.

Abstract ID: 779

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Fiber reinforced Composites

Keywords: Fiber-reinforced composites, orthotropic materials, heat-flux, thermal stress intensity factors.

Study of thermally insulated pair of collinear interfacial cracks parallel to a third interfacial crack situated in a composite medium

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The article deals with the problem of thermal stresses produced due to the presence of multiple interfacial cracks in an orthotropic medium attributed to fiber-reinforcement in a uniform direction. The present mathematical model comprises three thermally insulated cracks all aligned with the fiber direction. It includes two collinear cracks in the upper interface parallel to a third crack in the lower interface of the composite medium. It is assumed that thermally insulated cracks are causing a disturbance for the steady-state uniform heat flow. By Fourier integral transform, the governing equations of motion are converted into two pairs of linear singular integral equations. These integral equations of the first kind with Cauchy type kernel functions are solved using Chebyshev polynomials. Numerical values of the Mode-II thermal stress intensity factors are found for different particular cases for the considered orthotropic materials viz., Graphite epoxy, E-Glass fiber, and E-Glass epoxy which are displayed graphically.

Abstract ID: 780
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Bio-composites
Keywords: Cellulose, Composite, Thermoplastic, Granule

Cellulose-based composite materials for additive manufacturing in in electrical insulation, automotive and marine industries

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As the awareness on resource sufficiency, climate change mitigation and circularity of materials increases globally, many industrial sectors are currently looking for novel solutions in replacing fossil-based materials. Cellulose as a nature-based, sustainable and versatile material is a potential replacement for many synthetic materials. In addition, cellulose has many unique inherent properties that make it interesting for novel type of applications, beyond the obvious ones, such as paper and board. However, when considering the combination of cellulose and additive manufacturing (AM), one challenge is painfully obvious: cellulose is not thermoplastic by nature.

This challenge is currently being addressed in an EU funded project NOVUM, eventually targeting at building a pilot line suitable for producing components from cellulose-based composite materials by AM for versatile applications. During the project lifetime, the process will be demonstrated for electrical insulation, marine and automotive industries. For electrical insulation components, cellulose is a common raw material but the state-of-the art production method is rather inefficient in terms of labor, time, energy and waste generation. Additive manufacturing presents an appealing technology for boosting the process. For marine industry, the use case would be something completely new - on-demand printing of outdoor decorative elements for cruise ships. For automotive industry, the key motivation is the increase in sustainability, which the replacement of fossil-based materials with bio-based ones will bring about.

The thermoplastic cellulose-based composite materials developed in the project contain cellulose derivatives, such as cellulose acetate propionate, microcellulose and bio-based plasticizers. They have a higher cellulose content (up to 60%) than the commercial references but the material strength properties are at the same level or even better. The material properties can be tuned according to the requirements of the end use. The materials have excellent printability using commonly available printing technologies such as Fused Deposition Modelling (FDM) and light and have a smooth surface. The composite materials can be printed as granules and there is a possibility for recycling and reuse of the material by crushing and granulating, without the need of compounding prior to printing, thus contributing to the circularity of the materials.

Abstract ID: 781
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Smart Composites
Keywords: hydrogel nanocomposite, photo-thermo actuation, radiation technology, soft robotic

Hydrogel nanocomposite photoactuator for direct optical to mechanical energy conversion obtained by ionizing irradiation

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The incorporation of suitable nanomaterials into the stimuli responsive hydrogel matrix enables the hydrogel nanocomposites to become a key soft component of new generation of soft electronic and soft robotic devices1,2. An energy transformation agent, functional gold nanoparticles and nanorods exhibit unique photo-thermal properties as a result of a surface plasmon resonance electron-phonon process and intrinsic inter-band transitions. Upon immobilization in thermo-responsive hydrogel, they induce local photo-thermal shrinking under visible light irradiation and thus enable external wireless remote control of hydrogel device and programmable photo-thermo-mechanical motion. In addition, in this way control of interface conductivity can be realized by switching hydrogel nanocomposites between electrically communicating and non-communicating states.

In this work, a soft photo/thermal reversible hydrogel nanocomposite device consisting of gold nanoparticles or nanorods embedded in poly(N-isopropylacrylamide) (PNIPAM) and poly(N-isopropylacrylamide) (PNIPAM)/poly(vinyl alcohol) (PVA) bilayer structure (in order to maximize shape changes), were developed using nanotechnology based on radiation chemistry. The key parameters deciding the actuation characteristics as well as conductivity and percolation threshold, particle diameter and shape as well as interparticle distance, can be easily tailored during synthesis using radiation processing technology. Obtained hydrogel nanocomposite device with wireless remote actuation and electrical control has great potential for light-harvesting and mechanical motion which is required for the construction of soft smart actuator systems for applications in soft robotics, for dense information storage and efficient energy conversion.

Abstract ID: 782
Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)
Invited Talk
Topics: Spintronics
Keywords: Spintronics materials; Van der Waals; stacking heterostructure

Van der Waals heterostructure by stacking engineering

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Van der Waals heterostructure by stacking engineering

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Van der Waals (vdW) materials have attracted extensive attention because of their impressive stable properties at atomic thickness. The interlayer vdW interaction in the 2D material uniquely allows building a vdW homo/hetero-structure by a layer-stacking means without the need for lattice matching,1, 2 superior to the conventional solid interface grown in vacuum generally suffering from various perturbations, such as defects,3 lattice mismatch,4 and atomic interdiffusion.5 Here, we demonstrate the novel spintronics properties, such as ferromagnetic-antiferromagnetic exchange bias effect in vdW heterostructures by stacking engineering, compared to that in conventional materials. Our work provides a path for the exploration of other novel physics such quantum anomalous Hall effect, topological superconductivity in two-dimensional heterostructure materials.

Key Words: Spintronic materials; Van der Waals; stacking heterostructure

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Abstract ID: 783
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Fiber reinforced Composites
Keywords: FRPs, Femtosecond laser, LIPSS, Superhydrophobic, Self-cleaning

Ultrafast laser micro/nano-structured multi-functional carbon fiber reinforced plastic composites for aerospace applications

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Carbon fiber-reinforced plastics (CFRPs) laminates are extensively used in the aerospace sector due to their high strength and stiffness, low weight, and better fatigue resistance [1]. However, machining-induced damages such as delamination, fiber rupture, fiber-matrix debonding, and high tool wear while using the conventional machining process need to be addressed prior to the usage of CFRPs for various applications [2]. Despite extensive research on replacing metals by CFRPs for weight reduction in aircraft applications, there are open issues such as ice accretion and adhesion that need to be investigated further [3]. Hence, opportunities exist to improve surface characteristics by functionalizing CFRPs using surface micro/nano-texturing [4]. A number of surface functionalization methods have been used earlier such as sol-gel, electrodeposition, lithography, chemical etching, and microreplication. However, ultrafast laser structuring of materials has been accepted as an excellent technique to functionalize the surface [5].

This work focuses on the micro/nano-structuring of the CFRP surfaces using a femtosecond laser. Process parameters were varied to produce laser-induced periodic surface structures (LIPSS) on the material. Melt-free and well-defined hierarchical structures are generated on the CFRP samples that have been characterized using a scanning electron microscope (SEM). Moreover, 3D-optical profilometry was performed to analyze the depth of produced structures. Wettability behavior was assessed by measuring static contact angles (SCAs). Furthermore, treated surfaces were coated with 1H,1H,2H,2H-Perflorodecyltrithoxy-silane to decrease the surface energy and achieve superhydrophobic behavior. Results indicate a significant increase in SCA along with self-cleaning characteristics after coating. The applicability of laser structured CFRPs surfaces as metamaterials is presently being investigated, and the results would be presented.

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Abstract ID: 784
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Smart Composites
Keywords: Stimuli-responsiveness, Pickering emulsions, bio sourcing, sustained release

Formulation and polymerization of Pickering emulsions stabilized by stimuli-responsive dextran-based nanoparticles

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Pickering emulsions offer outstanding kinetic stability, appreciable for storage. It is of great interest to confer them stimuli-responsiveness [1] for applications that often require release of the content. The aim of our work is to formulate Pickering emulsions stabilized by dextran-based stimuli-sensitive nanoparticles. To do so, we modified dextran: a bio-sourced, biocompatible and biodegradable hydrophilic polysaccharide in three different ways. Then, nanoparticles made of modified dextran exhibiting narrow size distribution (PDI<0.2) and average hydrodynamic diameter around 200 nm were produced using nanoprecipitation. The initial modification step provides wettability and ensures stimuli-responsiveness to pH, enzyme or light of these nanoprecipitated particles for their use in Pickering emulsion stabilization. Oil-in-water Pickering emulsions were successfully formulated using these three different types of nanoparticles and limited coalescence phenomenon was studied. Degradation of the nanoparticles and destabilization of the related Pickering emulsions under stimuli (pH [2], enzyme, or light (Figure 1)) were achieved, promoting new bio-friendly vectors for lipophilic substances. The next step is to polymerize the inner phase of simple Pickering emulsions.

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Abstract ID: 785

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Synthesis and characterization of Composite materials

Keywords: FT-IR, Raman, AFM-IR Imaging Spectroscopy, Biopolymer Blend, Phase-Separation

Visualization of Structural Details in Biopolymers: From Micrometer to Nanometer Scale

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This presentation focuses on structural investigations of biopolymer blends by vibrational spectroscopic imaging techniques that provide lateral resolutions ranging from micro- down to nanometers. Generally, bio-degradable polymers which are produced from raw materials of the agricultural production chain or by the action of microorganisms are rapidly gaining economic importance. This is due to the increasing demand for reducing the exploitation of fossil raw materials and recycling short-lived products such as food packaging. Notwith-standing their environmental advantages, such biopolymers must fulfill the same end-user requirements in terms of their thermal and mechanical properties as the standard plastics, which presently dominate the world market. However, frequently individual biopolymers do not fulfill these specifications and have to be blended with other biopolymers for the optimization of their properties. Dependent on the blend concentrations, such biopolymer mixtures can undergo phase-separation, which is the target structural parameter of the reported investigations.

In this context, polymer blends of bio-degradable poly(3-hydroxybutyrate) (PHB) and poly(L-lactic acid) (PLA)1 were analyzed by FT-IR, Raman and Atomic Force Microscopy (AFM)-IR imaging spectroscopy. Generally, vibrational spectroscopic imaging enables a detailed lateral and chemical visualization of the investigated samples. However, while the FT-IR and Raman spectroscopic imaging techniques2 are diffraction-limited and have lateral resolutions of – at best – a few micrometers and a half micrometer, respectively, the advent of the AFM-IR3 technique, that exploits the photothermal effect, launched spectroscopic imaging to the 10 nm resolution level with the additional benefit of topographic information.

The imaging results obtained from the above biopolymer blend will be discussed with reference to the structural details revealed by the techniques ranging from lower to higher lateral resolution (viz. FT-IR, Raman and AFM-IR spectroscopic imaging).

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Abstract ID: 786

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: Supercapacitors, Optical Effects, Thermal Effects, Nano, Energy Storage

Optically Controlled Supercapacitors with Semiconductor Embedded Active Carbon Electrodes

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Supercapacitors, S-C - capacitors that take advantage of the large capacitance at the interface between an electrode and an electrolyte - have found many short-term energy applications. We concentrate here on optically induced, electrical and thermal effects. The parallel plate cells were made of two transparent electrodes (ITO), each covered with semiconductor-embedded, active carbon (A-C) layer. While A-C appears black, it is not an ideal blackbody absorber that absorbs all spectral light indiscriminately. In addition to relatively flat optical absorption background, A-C exhibits two distinct absorption bands: in the near-IR and in the blue. The first may be attributed to absorption by OH- group and the latter, by surface plasmons. The near IR absorption band mostly contributed to thermal effects, whereas the incorporation of blue absorbing nano-Si particles, resulted in a substantial capacitance increase under moderate light illumination [1]. Here, optical and thermal effects of micron size SiC particles that are embedded in A-C electrode, are presented. Similarly to nano-Si particles, SiC exhibits blue band absorption, but it is less likely to oxidize. Comparisons between the various capacitor constructions were based on the relative capacitance change, □C/C=(Clight-ON/Aexposed-Clight-OFF/A)/(Clight OFF/A). The expression takes into account the smaller light exposed area of the ITO electrode, Aexposed, with respect to the overall ITO electrode area, A. □C/C for SiC embedded particles is quite large (~30%) but not as large as for nano-Si embedded electrodes (which could reach 100%). As to the optically induced thermal effect, their contribution were found to be relatively small in comparison to the optically induced electrical effect. When analyzing these systems one may consider two processes: ionization of the semiconductor particles and charge displacement, or a dipole effect. These are all described by a simple model to be presented. For example, a dipole formed in the optically excited particle draws more charges to the current collector, hence increasing the cell capacitance (conditional artificial dielectrics). Finally, other electrode doping have been considered: dye materials (Rhodamine B, Stilbene 420) and quantum dots (CdSe, CdSe/ZnS).

Key Words: Supercapacitors, Optical Effects, Thermal Effects, Nano, Energy Storage

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Abstract ID: 787

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Photonic devices and applications

Keywords: Upconversion, Heavy-atom-free, Metal-free, Triplet Sensitizer

Photon upconversion based on heavy-atom-free thiosquaraines

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Photon upconversion through triplet–triplet annihilation is of interest for a variety of applications, notably as a potential path toward exceeding the Shockley–Queisser limits for solar cells. We demonstrate a completely heavy-atom-free red-to-yellow triplet–triplet annihilation (TTA) photon upconversion system using a thionated squaraine sensitizer, both in fluid solution and in a solid-state composite architecture. Our thiosquaraine exhibits an intense red absorption band, no measurable room-temperature fluorescence, and a native triplet lifetime on the order of 20 μs. This triplet excited state is readily quenched by triplet energy transfer to rubrene as a model upconversion emitter. Selective 685 nm excitation of the thiosquaraine in the upconversion samples results in upconverted rubrene fluorescence centered at 570 nm. The system also exhibits upconversion under filtered red (650 nm long-pass) simulated solar illumination. We also apply this thiosquaraine to demonstrate red-to-yellow photon upconversion in a solid-state polymer composite, a prerequisite for light-harvesting device integration. In contrast with traditional TTA upconversion photosensitizers that require cost-prohibitive precious metals or photodegradable arylhalide groups, we present an easily-tunable squaraine dye that serves as a promising red-absorbing heavy-atom-free upconversion sensitizer for increased scalability and photostability. Our results demonstrate that thionated squaraines provide an exciting new platform for developing heavy-atom-free upconversion systems.

Abstract ID: 788

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: MoS2, nanoribbons, manipulation, assembly, electrical characterization

Molybdenum Disulfide Nanoribbons: Fabrication, Manipulation, Assembly and Beyond

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In the past decade, molybdenum disulfide (MoS2) has received intensive attention owing to its unique physical and chemical properties that enable applications ranging from optoelectronics to catalysis, energy storage, and environmental remediation. Being capable of manipulating MoS2 nanostructures and assembling them at designated locations as building blocks for advanced devices is essential for realizing their applications. Herein, we report an innovative and robust approach to synthesize large-scale MoS2 nanoribbons with tunable dimensions. The strong shape anisotropy of the long-shaped MoS2 allows intense electric polarization that endows them with facile manipulation with the electric tweezers based on combined AC and DC fields. The nanoribbons transport following prescribed patterns with precision positioning and angular control; they rotate both clockwise and counter-clockwise at different AC frequencies. Such a versatile manipulation of MoS2 (or any 2D materials) has been reported for the first time. Furthermore, the mechanical electrorotation behaviors of the MoS2 strongly correlate to their electronic type that supports their semiconductor nature. This is further confirmed by their rapid optoelectronic response to light from 450 nm to 750 nm. In parallel, owing to the polycrystalline nature of the MoS2 nanoribbons that carry abundant surface defects, they can be readily functionalized and assembled between microelectrodes with UV-light-triggered click-chemistry and remove Mercury from water efficiently. Overall, this research unveiled an innovative synthesis, manipulation, and assembly scheme of MoS2 that could be applied to various 2D transition metal dichalcogenides (TMD).

Abstract ID: 789
Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)
Invited Talk
Topics: Photonic devices and applications
Keywords: Quantum cascade lasers, superlattice, van der Waals structures

Van der Waals structures make near-IR quantum cascade lasers

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Quantum cascade lasers (QCLs) constitute a leading source of coherent radiation in the mid-infrared region. However, their performance outside this region remains unsatisfactory. Indeed, there are currently no QCLs in the near-Infrared (near-IR) region. I propose that a superlattice of atomically thin layers held together by van der Waals forces can operate as a compact and powerful room-temperature near-IR QCL emitting at wavelength 1.66 μm. It can compress over 100 stages within 0.5μm. The electric field required for operation is about 3×106V/cm, while the lasing threshold current density is about 22.4kA/cm2 depending on parameters. Rate equation analysis shows that the peak power per unit volume can reach over 0.1mWμm−3 in continuous wave (c.w.) operation. Unlike most existing QCLs, our device is p-type working with holes designed with an unusual injector.

Abstract ID: 790

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Electrical properties of graphene, Mxenes and other two-dimensional materials

Keywords: Transfer-free monolayer graphene, Low-temperature growth, Giant domain size, High-conductivity, Superb-stretchability

Direct Growth of Highly Conductive Large-Area Stretchable Graphene at 100 oC

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The direct synthesis of inherently defect-free, large-area graphene on flexible substrates is a key technology for soft electronic devices. In the present work, in situ plasma-assisted thermal chemical vapor deposition (PATCVD) is implemented in order to synthesize 4-inch-diameter high-quality graphene directly on 10-nm-thick Ti-buffered substrates at 100 °C. The in situ synthesized monolayer graphene displays outstanding stretching properties coupled with low sheet resistance. Further improved mechanical and electronic performances are achieved by the in situ multi-stacking of graphene. The 4-layered graphene multi-stack is shown to display an ultralow resistance of ~ 6 □ per square, which is consistently maintained during the harsh repeat stretching tests and is assisted by self-p-doping under ambient conditions. Graphene-field effect transistors fabricated on polydimethylsiloxane (PDMS) substrates reveal an unprecedented hole mobility of ~ 21,000 cm2V-1s-1 at a gate voltage of -4V, irrespective of the channel length, which is consistently maintained during the repeat stretching test of 5,000 cycles at 140% parallel strain.

Abstract ID: 791

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Dielectric materials

Keywords: time-varying, Relation dispesion, permittivity, permeability, Transmission line

Electromagnetic Wave in Time-Modulated Material Media and Transmission Lines

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We briefly review the work done by our group on wave propagation are systems that are periodically modulated in time: a dielectric slab with modulation of its permittivity, a magneto-dielectric slab with simultaneous modulations of both permittivity and permeability, and a low-pass transmission line with modulation of its capacitance. We have predicted band gaps in the wave vector k (or propagation constant), frequency combs in the transmitted and reflected light, parametric resonances that depend crucially on the size of the slab, and strong interactions between the electric and magnetic modulations.

Abstract ID: 792

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Magneto Electronic Materials

Keywords: Multiferroics, M-type hexaferrites, Antiferroelectricity, Ferroelectricity, Magnetic semiconductor.

Multiferroism of La Modified M-type Hexaferrites

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Ferroelectric polarization and magnetic properties in La modified M-type hexaferrites (LaMFe12O19) will be presented, together with some antiferroelectric characterization of heavily doped ferrites. The remnant polarization of the LaMFe12O19 ceramic is more than 100 μC/cm2, exhibiting large spontaneous polarization double hysteresis loops at room temperature. Subsequent annealing of the LaMFe12O19 ceramics in oxygen atmosphere plays a key role on the saturation of its polarization hysteresis loop due to the great enhancement of its electric resistance. Two current peaks in I-V curve reveal the switching of polarization. The abnormal variation of dielectric constant near the Curie temperature (above 450C) demonstrates two phase transition peaks of ferroelectric to anotiferroelectric and antoferroelectric to para-electric phases. All these experimental results provided enough evidences to confirm the intrinsic ferroelectricity of M-type hexaferrites. Strong ferromagnetic performance was existing in this compound as usual. The origin for the coexistence of ferroelectricity and ferromagnetism in one single compound of M-type hexaferrite will be discussed in detail from the point of view of atomic structure. Large magnetoelectric coupling effect in the LaMFe12O19 ceramic specimens, appearing as spin current waves, will also be presented. The electronic transportation performances at low and high temperatures as well as magnetic semiconducting feature will be included in the presentation. The combination of ferroelectricity and ferromagnetism provides us an opportunity to fabricate novel multiple phase memories for info storage and quantum communication.

Abstract ID: 793

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Sensors and MEMS: Materials and Devices

Keywords: Semiconductor diamond, Electronics, MEMS, sensors

Semiconductor Diamond Electronics and MEMS sensors

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Diamond with an ultra-wide bandgap 5.5 eV shows potential performance that is extraordinarily superior to those of the currently available wide-bandgap semiconductors for energy-saving electronic and microelectromechanical systems (MEMS) devices. For example, the ultra-wide bandgap of diamond enables a high blocking voltage switching devices, and the low mechanical loss offers mechanical resonators with ultra-high quality (Q) factors for sensing applications. For power devices, from the viewpoint of low energy loss, safety aspects, gate reliability, and electronic circuit simplicity, normally-off field-effect transistors (FETs) with low subthreshold slope (SS) values and tunable threshold voltages are strongly in demand. Junction FET by using p-n junction or Schottky metal gate is the traditional method to achieve normally-off operation. Nevertheless, n-type dopants with shallow energy levels in diamond is notoriously difficult. While for metal-semiconductor FETs (MESFETs), there is an intrinsic problem of forward bias limitation.

Here, we propose and demonstrate a device concept of metal-insulator-metal-semiconductor FET (MIMS-FET) based on p-type diamond surface channel to overcome the drawbacks of MOSFET and MESFET. On the other hand, we developed single crystal diamond (SCD)-on-SCD MEMS resonators with ultra-high Q factors over 1 million by using a smart-cut method. We describe a robust and high-performance on-chip SCD NEMS/MEMS by proposing a transduction scheme called self-sensing enhancing actuation (SEA) with integrated actuation and sensing. Diamond MEMS magnetic sensor is also reported in this talk.

Abstract ID: 794

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Computational modeling and simulation for energy storage and conversion devices
Keywords: M3I3, Materials Imaging, Machine Learning, Data Mining, Structure-Property, Processing-Structure

Materials and Molecular Modeling, Imaging, Informatics and Integration (M3I3)

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M3I3 is an algorithm to perform a reverse engineering of future materials. Fast followers usually copy the first movers' products by reverse engineering them. For example, in case of the state-of-the-art battery products, the competitors dissect them into pieces and analyze the structure and composition of each part such as cathode, anode, electrolyte and separator. This so called "reverse engineering" is the cheapest way to catch up with the forefront runners in the ever-expanding competing world. For the front-runners, they also need a way to defend themselves and aggressively keep the distance from their competitors, and that's why they invest a huge amount of resources into research and development of new materials, devices, systems and platforms, and file patents all over the world. M3I3 provides a means to achieve this goal effectively by mimicking "reverse engineering" strategy with a higher level of creativity. M3I3 reverse engineers future materials of interest with superior performance and reliability as well as with minimum cost and environmental impact.

How is this possible? Reverse engineering starts from analyzing the structure and composition of the cutting-edge materials or products. Once we determine the performance of our targeted future materials, we need to know the candidate structure and composition of the future materials. This knowledge can only be available if we know the structure-property or the property-structure relationship of all materials and molecules at all scales. High-quality multi-scale and multi-dimensional experimental data will the key to the success of our approach. But there are critical challenges such as collecting and analyzing those data with consistency.

We hope to address those challenges during the workshop and form a clearer idea for our future direction.

Key Words: M3I3, Materials Imaging, Machine Learning, Data Mining, Structure-Property, Processing-Structure

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Abstract ID: 795

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Carbon/Carbon Composites

Keywords: carbon, fibers, flakes, thermal, management

Manufacturing and characterization of carbon fiber reinforced Aluminium metal matrix composite

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In today's advanced electronic world, for efficient and reliable working of electronic components, heat must be quickly dissipated for which very efficient heat sinks as well as electronic packaging materials are needed. Pure metals like Cu, Al, Au, Ag or combination of Cu-Mo, Cu-W can be the candidates due to high TC but they have high CTE as well. High density (except Al) and high cost are other important factors that inhibit their use. In carbon fiber reinforced AMMCs such combination can be tailored. Due to their light weight, high strength and good thermal properties, carbon fiber reinforced aluminium metal matrix composites (AMMC) are potential materials for aerospace components and also for thermal management in electronic components. We manufactured carbon fiber and flake reinforced composite with AA7075 as matrix ,and different volume contents of carbon fibers and graphite flakes as reinforcement. Effects of volume content of fibers /flakes on mechanical, thermal, electrical properties of composites were studied. Corrosion behavior of these composites was also studied. Metallographic examination was carried out using common techniques. By varying the amount of reinforcement, properties such as thermal, mechanical and electrochemical behavior were optimised. Outcome of this study would be useful for the development of efficient heat sink and electronic packaging materials.

Abstract ID: 796

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Composite structural materials

Keywords: Edge Crack, Interface, SIF, Time-Harmonic wave, Composite Structure.

Study of an Interfacial Edge crack between dissimilar orthotropic half-planes

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This article deals with the study of an edge crack situated at an interface of two dissimilar orthotropic half-planes. Considered model is subjected to time-harmonic wave disturbance, where the mathematical model has been solved by applying the Integral transform and then the unknown functions have been determined using the Schmidt method. Approximate analytical expression for the stress intensity factor (SIF) of Mode-I has been obtained at the tip of the crack.

The numerical computations have been done using E-glass epoxy for upper half-plane and Graphite epoxy for lower half plane and effect of time- harmonic wave disturbance on the Composite structural materials has been studied. The graphical representation of SIF for various crack lengths and wave numbers has been depicted..

Abstract ID: 797

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Graphene, Mxenes and other two-dimensional materials for biomedical and healthcare applications

Keywords: MXene, mxene-polymer composite, Cationic polymer, fluorescence, Ti3C2

Fabrication of Polyethyleneimine conjugated fluorescent MXene nanosheets and its cytotoxic evaluation

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MXene is one of the most exciting 2D materials currently, which has incredible potential in various applications. In this work, we report Polyethyleneimine (PEI) conjugated MXene nanosheets, which are cationic in nature. PEI_Ti3C2Tx (PEI_MX) was produced by etching Ti3AlC2, ultrasonicated along with PEI, and then hydrothermally treated at 200 0C for 24 hours. PEI is a positively charged polymer containing repeating amine groups. The as-obtained nanosheets were characterized through XRD, AFM, TEM, UV-vis spectroscopy. The thickness of PEI conjugated nanosheet was found to be 2.63±0.85 nm compared to control 6.82±1.66 nm, proving its utilization both as a surfactant as well as a functionalizing agent. The use of polymer also assists in forming a stable aqueous dispersion. The small-sized nanosheets were found to be highly biocompatible and exhibited blue fluorescence. The photoluminescence of the 2D nanosheets enables them to be also utilized as cell labeling probes. The PEI_MX are highly scalable and their intrinsic NIR activity, fluorescence, small size, and cationic character can be applied for a variety of applications like cell imaging and photothermal therapy.

Abstract ID: 798

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Industrial applications of composite materials

Keywords: calcium carbonate, composite filler, kaolin. silica, solid tire trolly

Effect of composite filler on mechanical properties and material homogeneity in solid tire vulcanization for trolly

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Effect of composite filler on mechanical properties and material homogeneity in solid tire vulcanization for trolly.

Abstract. Filler is one of the most important materials used to make various types of rubber vulcanizate. The filler in the rubber compound-making process acts as an active filler to improve the mechanical properties of the vulcanisate, and acts as a volume-increasing filler to reduce production costs. The filler composites used in this study are specifically for solid trolly tires which are commonly used to move goods within the airport area. Solid tire rubber vulcanisate in this study used a filler composite consisting of silica as an active filler, kaolin and CaCO3 as a volume enhancer. The loading of filler composites on the rubber matrix in this study varied from 50 to 65 phr. The manufacture of rubber composites for solid tires is carried out through a process of chewing, mixing natural rubber with synthetic rubber Butadiene Nitrile Rubber, componding, and vulcanization. The vulcanization process is carried out at a temperature of 150 °C for 20 minutes. The data from the test results before and after aging show that the composite filler ratio has an effect on specific gravity, hardness, and abrasion resistance. The homogeneity of the material was scanned using a scanning electron microscope (SEM). The scan results show that the distribution of the material on the rubber vulcanized matrix is influenced by the ratio of the filler materialTo see the functional groups of solid tire rubber vulcanisate used Fourier transform infrared spectroscopy (FTIR).

Abstract ID: 799
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Nanocomposites
Keywords: CNT network, Buckypaper, Interphase, AFM PFQNM

Properties of Carbon Nanotube Buckypaper and Interphase

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Thin-film infiltrated Buckypaper (BP) is a membrane of high CNT content nano-composites, consisting of entangled CNT networks with a porous mesh structure infiltrated with a polymeric material. The interaction between the CNT network and the surrounding polymer and between BP and the surrounding polymer in a 3-phase nano-composite occurs via interphase. This study aims to investigate the heterogeneity of BP at the nano-scale and the homogeneity at the microscale. The author uses the Atomic Force Microscopy-based Peak Force Quantitative Nanomechanics Mapping (PFQNM) technique to study the CNT BP and the CNT network interphase at the nano-scale with high lateral resolution. The trace and retrace curves of force vs. deformation response will be analyzed using Derjaguin-Muller-Toporov and Johnson-Kendall-Roberts models. Biaxial carbon fiber, Bisphenol-A/F type epoxy with amine hardener, and nonfunctionalized multiwall carbon nanotube (MWCNT) with an average outer diameter of 10-30nm, an average length of 15-30µm were used to fabricate BP nano-composites. The histogram of reduced modulus, adhesion, and deformation will be examined to understand the heterogeneity of BP, and the homogenized values will be compared with the static test of BP films. The size of CNT networks will be studied via. AFM and SEM. The stochastic nature of the CNT network interphase with the surrounding polymer will be investigated.

Key Words: CNT network, Buckypaper, Interphase, AFM PFQNM

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Abstract ID: 800

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Model catalysts, Molybdenum-Boron surface alloy, alloy oxide, Carbon monoxide oxidation, surface sensitive techniques

Design of non-noble metal containing compounds as alternatives to noble metal catalysts: The MoxByOz ternary alloy for Pd (Pt, Au)

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In a search of alternatives to precious metal containing heterogeneous catalysts, it has been demonstrated previously that addition of submonolayer concentrations of boron to Mo(110) surface via alloying dramatically changes its adsorption and reaction properties for carbon monoxide and oxygen molecules in the way like that exhibited by precious metal catalysts [1]. The main effect is that the CO reaction pathway shifts from dissociation on bare Mo(110) to oxidation on borided Mo(110). This is due to specific state the boron atoms acquire at the surface, as well as to structural and electronic transformation of the substrate. In an attempt to get closer to performance exhibited by precious metal catalysts, the main focus of the present study was to find out how the (CO+O2) adsorption and reaction properties of the model borided Mo(110) substrate further change upon its oxidation. For this, an experimental investigation of a corresponding in-situ prepared model systems in an ultra-high vacuum condition with a set of complimentary surface sensitive techniques - XPS, TPD, LEIS, FTIR - has been done. The B-Mo (110) surface alloy was formed after annealing at a temperature of 1300 K of the system formed by depositing of 2 boron monolayers on the surface of Mo (110). The resulting alloy was oxidized by backfilling the UHV chamber with oxygen to a partial pressure of 10-6 Torr and subsequent annealing at 900 K for 10 min. The adsorption of carbon monoxide and oxygen molecules was carried out by inflowing the corresponding gases into the chamber to a partial pressure of 5 x 10-8 Torr, and a substrate temperature of 95 K. The oxidation of the B-Mo (110) alloy with a submonolayer concentration of boron atoms leads to a dramatic increase in the efficiency of the conversion of co-adsorbed carbon monoxide and oxygen molecules to carbon dioxide. This is due to the difference in the properties of adsorbed species before and after the oxidation of molybdenum boride, in particular, an increase in the tilt of the CO molecular axis to the plane of the adsorbent surface and weakening of the chemisorption bond of oxygen with the substrate on the surface of the MoxByOz ternary compound. This substrate can be viewed as a model system, alternative to existing catalysts for CO oxidation based on precious metals (Pd, Pt, Au).

This work was supported by the Goszadanie-2021 of Russian Ministry of Science and Higher Education

Key Words: Model catalysts, Molybdenum-Boron surface alloy, alloy oxide, Carbon monoxide oxidation, surface sensitive techniques

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Abstract ID: 801

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Topological Insulators, 2D Materials, and Voltage Controlled Magnetism

Keywords: Magneto-Seebeck effect, Bi2Te3

Magneto-Seebeck effect on Pd doped Bi2Te3 topological insulator

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Topological insulators constitute a class of quantum materials in the condensed matter physics with the conducting topological surface states and insulating bulk with a band gap. The first-generation three-dimensional topological insulators were confirmed experimentally in Bi2Te3, Bi2Se3 and Sb2Te3 which are well-known thermoelectric materials.[1] Since decades, Bi2Te3 have been known for highest thermoelectric figure of merit, ZT near room temperature applications.[2] Seebeck effect or thermopower has always been studied extensively to enhance thermoelectric figure of merit, ZT. We have studied magneto-Seebeck effect on single crystals of pristine n-type Bi2Te3 and doped PdxBi2Te3 (0 □ x □ 0.20) on a setup designed for Seebeck and Nernst effect measurements integrated with the physical property measurement system (PPMS) by Quantum design.[3] This study discusses the magneto-Seebeck and power factor with the Pd doping in Bi2Te3. Our findings of the change in sign of Seebeck effect from negative to positive with Pd-doping signifies change in carrier types from n to p-type has been verified through Hall effect and angle resolved photoemission spectroscopy (ARPES) measurements also.

Key Words: Magneto-Seebeck effect, Bi2Te3

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Abstract ID: 802
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Design and application of composite structures
Keywords: Cellular Tower, Fan Palm Stalk, Fiberglass

Design of a lightweight fiberglass stalk for a 'fan palm' camouflaged cellular tower

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In the current era, mobiles phones have become a necessity for many people worldwide. The increasing mobile phone usage has fuelled demand for a large number of cellular towers. However, people do not want a telecommunication tower erected in their locality as it ruins the landscape. So, the telecommunication companies have come up with the idea of camouflaged cellular towers. Despite being a brilliant idea, the existing 'fan palm' camouflaged cellular towers in Mauritius are not widely appreciated because they are far from resembling natural trees and are not durable enough. The artificial 'fan palm' stalk is made of high molecular weight polyethylene and the lack of flexibility of the structure makes it prone to crack formation and even breakage under bending or twisting caused by strong winds. Failure of the stalk can cause casualties and also damage the antennas, thus affecting signal transmission. In this study, the redesign of the stalk of such a camouflaged tower has been inspired by a natural 'fan palm' stalk. Given its high modulus of rupture and good tensile strength, the RF transparent fiberglass material has been chosen for the stalk. The geometrical features of a natural 'fan palm' stalk, such as cross-sectional area and shape, have been replicated in the artificial one such that the latter behave naturally. The stalk should be flexible so that it can swing like a natural one. This has been achieved through shape optimization and weight reduction of the stalk. A 3D model of the stalk has been created in Solidworks and the stress induced under cyclonic wind conditions has been analyzed by performing a structural static analysis in Ansys Workbench. It has been observed that the nature-inspired shape of the stalk has a huge impact on increased durability and flexibility of the structure.

Abstract ID: 803

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Optical properties of metals and non-metals

Keywords: double perovskite, atomic substitution, X-ray photodetectors, tuning optoelectronic properties.

Tuning Structural and Optoelectronic Properties of Lead-free Double Perovskites through Alkali Substitution

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The discovery of lead halide perovskites as suitable materials for optoelectronic applications is considered as a milestone in solar cell research. Despite their meteoric rise, major issues hinder their use in commercial applications such as the toxicity of lead and their inherent instability towards moisture.

We present the results of a comprehensive study targeting the structural and opto-electronic properties of lead-free double perovskite single crystals based on the compound Cs2AgBiBr6. Previous studies have shown that double perovskites are stable and nontoxic alternatives for lead-based perovskites. Cs2AgBiBr6 has emerged as a promising material with suboptimal photon-to-charge carrier conversion efficiency, yet well suited for high-energy photon detection applications.

In order to alter and optimize the optoelectronic properties of this compound, we have substituted the Cs cation by the alkali metals, Rb, K and Na [Adv. Mater. 2020, 32, 2001878]. We show results on the optoelectronic and structural properties of pure Cs2AgBiBr6 and alkali metal substituted (Cs1-xYx)2AgBiBr6 (Y: Rb+, K+, Na+) single crystals and demonstrate that alkali substitution enhances electron-acoustic phonon scattering. Although, the nature and size of the bandgap remains unchanged upon alkali-substitution revealed by absorption and steady-state photoluminescence, the fundamental carrier recombination lifetime is greatly enhanced. Moreover, from thermal expansion measurements we find that alkali-substitution alters the phase transition temperature between the low-temperature tetragonal and the high temperature cubic phase. Strikingly, alkali-substitution entails a tunability to the material system regarding the response to high-energy photon detection: their response upon X-ray exposure drastically changes hence, their X-ray sensitivity outperforms other double perovskite-based devices reported.

Altogether, we present new pathways to apply alkali-substitution as an engineering tool to tune the properties of double perovskites towards a new material platform for optoelectronics.

Abstract ID: 804

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Optical properties of metals and non-metals

Keywords: Electrochemical SERS, Electron transfer, Electronic structure, DFT calculations

A non-trivial view of the metal-molecule electron transfer: Chemical, electrical and photonic factors

Samuel Valdivia, Daniel Aranda, Francisco J. Avila-Ferrer, Isabel López-Tocón, Juan Soto, Juan Carlos Otero

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This communication deals with the properties of molecules bonded to charged metal surfaces (electrodes, nanostructures or clusters), especially focused on the charge transfer (CT) process. The energy requirements for forward (F-CT: metal-to-molecule) and reverse (R-CT: molecule-to-metal) electron transfer are usually explained on the basis of very popular schemes based on the relative position of the Fermi level (FL) of the metal with respect to the energies of the LUMO (F-CT) or the HOMO (R-CT) orbitals of the molecule (Fig. 1). The electrode potential (EV) is a key parameter given that, for instance, negative shifts (-EV) raise FL and, therefore, reducing EF-CT and increasing ER-CT, respectively: -eEV=-EF-CT=ER-CT.

In such scheme metal and molecule are not “connected”, the only role of EV is to shift FL. Several photoelectrochemical experiments do not support this trivial energy conversion G=ECT/EV=1 eV/V. Experimental G values are very scattered but shows unexpected huge energy gains (G=3-5 eV/V [1]) which can be explained on the basis of theoretical calculations. DFT calculations on charged metal-molecule hybrids are able to explain the complex dependence of the properties of the interface on the chemical nature of their constituents and on the subtle effect of applied potentials giving huge [1] or zero energy gain [2], depending on the strength of the surface complex. The metal-molecule hybrid system has two different electronic structures which are selected by the sign of the surface excess of charge of the metal. Besides G values, this dual electronic structure shows a sharp change in other properties as the dependence of the adsorption energy or the vibrational wavenumbers on the applied voltage.

Abstract ID: 805

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Optical properties of metals and non-metals

Keywords: Electrochemical SERS, Electronic structure, DFT calculations, interfaces

How the electrode potential selects the dual electronic structure of charged metal-molecule interfaces: Surface-enhanced Raman scattering of cyanide adsorbed on nanostructured silver electrodes

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Experimental and theoretical calculations confirm the existence of two different electronic structures of a surface complex formed by a particular molecule bonded to charged metal electrodes, clusters, or nanoparticles. Each electronic structure of the metal-molecule hybrid system is selected by sign of the surface excess of charge of the metal at potentials more negative or positive than its potential of zero charge (PZC).

Surface-enhanced Raman scattering (SERS) of cyanine adsorbed on a silver electrode shows two regions, which are selected by the voltage and characterized by the differentiated response of the vibrational wavenumbers of the ν(CN) stretching band. The combination between the experimental SERS and theoretical DFT calculations has allowed for relating the two regions to chemisorbed (C-hybrid, region A) and physisorbed (P-hybrid, region B) surface complexes, where cyanide is bonded through the carbon on top of a single silver atom of the surface. The electrode potential selects one or another type of electronic structure of the system, which are of different nature having a differentiated response to the applied voltage. The electric potential tunes smoothly the wavenumbers, bond energies, and injected charges of the P-hybrid at more negative potentials than PZC, but the very strong C-hybrid prevents significant changes of these properties at positive excesses of charge. The existence of the dual electronic structure of metal-molecule interfaces might require reinterpreting experiments that are usually discussed by resorting to, for instance, the reorientation of the adsorbate, the formation of complexes with different stoichiometries, the existence of nonequivalent local sites on the surface, or to instrumental artifacts. Moreover, this dual behavior also determines the properties and responses of technological devices where metal-molecule interfaces are involved.

Abstract ID: 806

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Taylor vortex flow, Couette-Taylor reactor, flow pattern, CuPd alloy nanoparticles, dispersion

Dispersion Control using Taylor-Vortex Flow in the Synthesis of CuPd Alloy Nanoparticles

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In the catalytic reaction, it is very important to synthesize well-dispersed and small-sized nanocatalysts to obtain a high catalytic surface area. In this study, a facile new synthetic method to control the size and dispersion of nanoparticles by controlling the flow pattern in the reactor is first reported. A Couette-Taylor (CT) reactor is capable of generating regular and strong flow throughout the reactor. This regular and strong flow increases the reaction rate in the synthesis of nanoparticles to make the size smaller, and promotes the progression to the dispersion state rather than the aggregation state, enabling the formation of small and independent nanoparticles. Using a continuous CT reactor, CuPd alloy nanoparticles with sizes of less than 5 nm were easily synthesized. In high rotation speed of 1200 rpm, nanoparticles did not form aggregation and exist independently and stably, while only aggregates were observed in the mixed tank (MT) reactor. We also investigated the effect of various factors such as rotating speed, mean residence time, and concentration of reagents and stabilizer on the size and dispersion of CuPd alloy nanoparticles.

Abstract ID: 807

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Energy release rate, Fracture testing, Finite element analysis, Magnetoelasticity, Terfenol-D epoxy composite

Experimental and Numerical Analysis of Influence of Magnetic Field on Critical Fracture Parameters of Terfenol-D Epoxy Composite

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Modern smart materials such as Terfenol-D epoxy composites have a wide range of applications, particularly in high-frequency sensors and actuators. The Terfenol-D epoxy composites are brittle in nature and susceptible to fracture during high-frequency operations. This work experimentally and numerically characterizes Terfenol-D epoxy composites' fracture behaviour subjected to an applied magnetic field. The three-point bending fracture tests have been carried out using single edge notch bend (SENB) specimens as per ASTM standard D5045-14 to estimate the fracture load and critical fracture parameters K_Ic, G_Ic, J_Ic using the digital image correlation technology in the presence of the magnetic field at different loading rates. A plane strain finite element analysis (FEA) was also conducted, and the effect of magnetic field on the critical energy release rate was elaborated in detail. In FEA, a vector generalized nonlinear constitutive relations are used to incorporate the nonlinear elastic strain and ΔE effect induced due to the magnetic domain rotations caused by stresses. Experimental and numerical fracture parameters are compared quantitively and qualitatively to describe the significance of nonlinearity in strain. Additionally, fracture surfaces are inspected by using scanning electron microscopy to corroborate the fracture characteristics.

Abstract ID: 808

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Electrochemical Supercapacitors

Keywords: Supercapacitors, Phosphorus@MXenes compact films, 3D chemically bonded porous network, Energy storage

Chemically Bonded 3D Porous Network of Black Phosphorus@MXenes Enables High and Stable Capacitive Energy Storage

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The performance of supercapacitors is largely limited by the lack of high-mass-loading electrodes (~10 mg cm-2) and therefore they offer relatively low volumetric energy density, where there is an increase in limit of ion diffusions with thickening in film electrodes. We have developed a rational design for black phosphorus@MXenes compact films of 3D chemically bonded porous network structure. They are successfully made by in-situ growth of black phosphorus (BP) nanoparticles on 2D Mxene, and give rise to a commercial-level capacitive energy storage at high mass loading (>10 mg cm-2). The strong chemical bonds (Ti-O-P) formed between BP nanoparticles and 2D Ti3C2 stabilize the 3D porous network structure, and therefore enable sufficient charge transports and electron environment for electrolyte ions absorption and storage. The 3D network porous structure formed by incorporation of BP nanoparticles into 2D Mxene further facilitate highly reversible ion adsorption reactions that contribute fast charging/discharging capability. The BP@Ti3C2 compact film electrode delivers an impressive volumetric capacitance of ~350 F cm-3, which is among the best performance ever reported so far for MXene-based SCs employing ionic liquid electrolyte. The supercapacitors made use of the BP@Ti3C2 compact film electrode with a mass loading of ~15 mg cm-2) offers a high stack volumetric energy density of >70 Wh L-1. We have conducted thorough investigations into the rationally designed 3D porous network structure of BP@Ti3C2 with chemical bonds between the two, and the key working principles are revealed.

Abstract ID: 809

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Photonic devices and applications

Keywords: Photonic crystal, Phosphor, Photonic band-edge, Colloidal quantum dot

Two-dimensional photonic crystal as a phosphor platform for efficient color conversion

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The importance of phosphors has been revived with the emergence of phosphor-capped white LEDs that triggered the display and solid-state lighting industries. While the mainstream phosphor development has been materials-oriented so far, the authors' group proposed photonic crystal (PhC) phosphors, a paradigm-shifting concept in phosphor research. The basic idea is to structurally engineer phosphor materials into a periodic PhC structure such that the associated □-point photonic band-edge (PBE) modes are tuned to phosphor excitation wavelength to induce an enhancement in color conversion efficiency. The employment of Γ-point PBEs, where the lateral momentum and group velocity are zero, is important because they allow the PhC structure to resonate with excitation photons impinging in the surface-normal direction. A two-dimensional (2D) square-lattice PhC structure has been identified as the most advanced PhC phosphor format, which is schematically shown in Fig. 1, where the PhC backbone layer (Si3N4) is sandwiched between a phosphor material (colloidal quantum dots; CQDs) and a transparent substrate (fused quartz). The square-lattice PhC removes the polarization sensitivity of excitation photons that the previous one-dimensional version of the PhC phosphor suffers. Further attempts to improve the performance of the PhC phosphors are under pursuit.

Abstract ID: 810

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Optical properties of metals and non-metals

Keywords: Thin film, Perovskite, Fluorescence

High-performance fluorescence sensing of Er:BaTiO3 thin films: a study by confocal scanning microscopy

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Ferroelectric thin films with luminescent properties applied as photonic devices require not only high linear and non-linear electro-optical coefficients [1,2], but also the bandwidth that gives high-performance for the near-visible infrared response. Barium titanate (BaTiO3) films doped with Er atoms with concentrations of 3 mol % (BT:Er) were grown on Pt/Si(100) substrates by spin coating. The crystallinity and morphology of the BT:Er films were characterized by the X-ray diffraction analysis and SEM, respectively. The ferroelectric and fluorescence properties of the BT:Er films were measured at room temperature. Polycrystalline BT:Er films with the tetragonal phase were grown, in which the Er concentration was kept less than 3 mol %. The remnant polarization value of the ~230-nm-thick BT:Er films with Er concentration of 3 mol % was approximately 0.86 μC/cm2. The fluorescence properties were evaluated by performing the up-conversion of the luminescence of the BT:Er thin films, using the Confocal Fluorescence Microscopy (CFM). Green and red up-conversion emissions at 520, 550 and 670 nm were observed from the BT:Er films with the excitations of 790, 800 and 980 nm. The fluorescence results suggest a clear dependence of excitation wavelength on the emission intensity, where a ~3-fold enhancement in emission has been demonstrated under Er3+ (800 nm) excitation which can be attributed to an effective energy transfer between the Er3+ ions.

Key Words: Thin film, Perovskite, Fluorescence

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Abstract ID: 811
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Bio-inspired design of composites
Keywords: cephalopods, bioinspired, camouflage, thermal management

Dynamic Materials Inspired by Cephalopods

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Cephalopods (e.g., squids, octopuses, and cuttlefish) have captivated the imagination of both the general public and scientists alike due to their sophisticated nervous systems, complex behavioral patterns, and visually stunning camouflage displays. Given their unique capabilities and characteristics, it is not surprising that these marine invertebrates have emerged as exciting models for novel adaptive optical and photonic materials. Within this context, our laboratory has developed various cephalopod-derived and cephalopod-inspired systems with tunable functionalities within the visible and infrared regions of the electromagnetic spectrum. Our findings hold implications for next-generation adaptive camouflage devices and energy conservation technologies.

Abstract ID: 812

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Functional Magnetic Materials

Keywords: Nanostructures, nanomedicine, magnetism

Vortex nanostructures: from micromagnetic simulations to cancer cells internalization for magneto-mechanically induced damage applications.

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Novel magnetic nanostructures (MNS) present a unique spin arrangement in the magnetic ground state, namely spin-vortex or synthetic antiferromagnetic state. They are not spherical, rather disc or wire-shaped. MNS showed promising results in cell separation, as a contrast enhancing agents in MRI and in magneto-mechanically induced cell annihilation. The main advantages of magneto-mechanically induced cell annihilation are the usage of weaker magnetic fields with lower frequencies, as well as the need for a lower concentration of particles [1].

In this work, we developed one subset of biocompatible magnetic nanostructures that exhibit a spin-vortex state with interest in analysing their application in magneto-mechanically induced cell death. First, micromagnetic simulations, using mumax3 of sub-micron iron discs, were performed for different interdot distance and aspect-ratio (thickness/diameter). By analysing the nucleation and annihilation fields, as well as the magnetic susceptibility, it was found that the (ideal) discs could be considered as isolated for interdot distances greater than twice the radius of the disc (2R) [2]. We also found that discs with an aspect ratio between 5 and 15 should sustain the vortex state in remanence.

Iron nano-discs, with a diameter of about 500 nm, were fabricated by electron beam evaporation on a Si substrate pre-patterned by interference lithography [3]. The discs, protected by bottom and top gold layers, were fully characterized and the obtained magnetic measurements are in good agreement with the micromagnetic simulations. Then, the magnetic vortex nano-discs were released from the substrate by chemical etching of a sacrificial layer. Subsequently, cell viability and uptake assays were performed in a human leukaemia monocyte cell line (THP-1). Several concentrations of nano-discs were studied by flow cytometry. As a result, the discs were internalized by the cells and found to be innocuous to them, in the absence of an external magnetic field.

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Abstract ID: 813

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Non-destructive Inspection Techniques for Composite Materials and Structures
Keywords: Ultrasonic guided waves, Electromechanical impedance, Composites, Damage analysis, Signal processing, Sensor networks, Piezoelectric transducers

Damage assessment of composites using techniques based on guided waves and electromechanical impedance

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In the presented research the guided waves (GW) propagation as well as the electromechanical impedance (EMI) were studied in the context of non-destructive evaluation (NDE) and structural health monitoring (SHM) of structural parts made of composites. Both techniques are employing piezoelectric transducers for actuation the structure and sensing the response. The focus in this research was put on relatively thin walled structural parts made of carbon fiber reinforced polymers (CFRP) as well as glass fiber reinforced polymers (GFRP). Multi-modal nature, dispersion, and direction dependence of guided waves propagation was considered for developing the damage detection tools. The results present the behavior of the waves influenced by the reinforcing fibers orientation, presence of the stiffener, as well as the presence of the damage. Moreover, in order to study the wave prorogation phenomenon in detail, the scanning laser Doppler vibrometer (SLDV) was employed allowing to visualize the whole wave field of the propagating waves. In the area of electromechanical impedance the range of sensitivity was studied and the effective frequency range needed for the damage assessment. Both techniques analyzed in this work depend greatly on the sensor placement on the inspected object. This topic was addressed by considering representative examples of sensor networks and performing damage localization using them. The signal processing procedures developed for damage assessment were analyzed and the advantages and disadvantages of the procedures were highlighted.

Abstract ID: 814
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Porous and cellular materials
Keywords: Aerogels, thermal insulation, waste recycling

Ambient drying of large, monolithic aerogels and aerogel composites

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Aerogels are generally thought of as materials that are difficult to process, fragile, and expensive. The mail processing and cost hurdle is their drying. Aerogels are typically dried in supercritical CO2, whose high pressure (72.8 atm) requires use of unwieldy, expensive autoclaves. Over the years, alternatives to supercritical drying have been developed, such as freeze- and ambient-drying. These techniques are less costly than supercritical drying, but they tend to yield materials in non-monolithic form. Here, materials produced by a proprietary ambient drying technique will be presented. These materials, which include transparent aerogels, and in some cases integrate waste products, have characteristics very comparable to those of aerogels produced by supercritical drying, and, most importantly, are monolithic. Implications for the building industry will be discussed.

Abstract ID: 815

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: Nitrogen-doped carbon, biomass, porosity, chemical activation

High performance nitrogen-doped porous carbons derived from biomass for supercapacitors electrodes

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This work studies a post-situ nitrogen-doped porous carbons prepared using a biomass waste, peanut shell (PS) as a carbon source and melamine as a nitrogen source. The synthesis method involved two steps mechanism, chemical activation of the peanut shell using KOH followed by nitrogen-doping of the porous carbon. The post-situ N-doped porous carbon with an optimum amount of KOH to PS exhibited the best capacitance performance with a specific surface area (SSA) of 1442 m2 g-1 and an enriched nitrogen content (3.2 at %). The fabricated symmetric device exhibited a specific capacitance of 251.2 F g-1 at a specific current of 1 A g-1 in aqueous electrolyte (2.5 M KNO3) at a wide range cell potential of 2.0 V. The cell delivered a specific energy of 35 W h kg-1 with a corresponding specific power of 1 kW kg-1 at 1 A g-1 . Moreover, long term stability of the device showed 83.2% capacity retention over 20 000 charge/discharge cycles and a good rate capability after 180 h of floating at 5 A g-1. This great performance of the symmetric supercapacitor can be correlated to the surface porosity and nitrogen doping effect, which increased the active sites for electrochemical activities.

Abstract ID: 816

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster/Oral Presentation

Topics: Anodes and cathodes Materials
Keywords: MXene, Rechargeable Mg Batteries, Energy Storage

Rechargeable Magnesium Battery Cathodes Based on Fluorine-free MXenes

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In order for rechargeable Mg batteries (RMBs) to compete with the energy density of today's Li-ion batteries, cathode materials with improved capacity and voltage must be realised.[1] Today's cathode materials suffer from either irreversible intercalation or insufficient energy density, which partly is due to the higher charge density of the divalent Mg-ions compared to Li-ions. One type of material that has been proposed as a possible candidate is the 2D MXene family, where the oxygen terminated vanadium based MXene, V2COx, has shown the highest intercalation energies and lowest migration barriers from DFT calculations.[2] Here, we report on a fluorine-free synthesis route for V2CTx MXene (T = O or OH) by an alkaline etching process. We also show how the material changes by various post-etching treatments. To verify the chemical and structural changes, EDS, XPS, XRD, SEM and Raman spectroscopy are utilized. The effect of the termination groups on the average potential and reversible capacity is experimentally determined and further discussed.

Abstract ID: 817

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster/Oral Presentation

Topics: Solar Cells

Keywords: Ultrasound, Silicon, Solar Cell, FeB pair

Ultrasound as Functional Influence Tool on FeB pair Association in Silicon Solar Cells

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Defects are crucial for solar cell (SC) performance. The irradiation and annealing are the widespread techniques of functional defect engineering. But another selective as well as room temperature realized way of defects modification is the ultrasound excitation in a crystal. The acoustic waves are able to cause redistribution of impurities, point defects rebuilding and affect SC properties as well [1]. In this work, the influence of ultrasound loading (USL) on a FeB pair association in silicon SC was under consideration. The iron is a major contaminant as well as one of the most detrimental impurities in silicon photovoltaic devices and the investigation is important from an applied point of view.

The Si-SC was fabricated from p-type boron doped wafer with <100> orientation and a doping level of 1.4 1015 cm-3. In USL case the longitudinal waves with 4.1 MHz frequency and up to ~0.5 W/cm2 intensity were exited. The FeB pair dissociation was made by halogen lamp illumination (0.25 W/cm2, 15 s). The short circuit current value (LED, 940 nm, 0.15 mW/cm2) was used to characterize recombination process in the SC base. The Isc kinetic was fitted by taking into account intrinsic recombination and to Shockley-Read-Hall recombination on interstitial iron and FeB pair and the iron atom migration energy Em was determined. The acousto-induced reduction in Em value has been revealed. The Em decrease runs up to 10 meV and non-linear depends on US intensity. Thus the ultrasound can be effective tool of defect engineering in solar cell functional materials. The work was supported by NRFU (project 2020.02/0036).

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Abstract ID: 818

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Nanostructured materials for advanced batteries

Keywords: Ferroelectricity, Energy Storage, Spectroscopy

Energy storage density in lead-free ferroelectric BaxSr1-xTiO3 thin films capacitor prepared using pulsed laser deposition technique

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Structure, phonon, and energy storage density in Sr2+-substituted lead free ferroelectric BaxSr1-xTiO3 (BST1-x) thin films for x = 0.1, 0.3, and 0.7, prepared using pulsed laser deposition techniques, were investigated using x-ray diffraction, Raman and ferroelectric polarization measurements as a function of temperature. The film is tetragonal for x =0.1 with large c/a ratio. The tetragonal anisotropy decreases upon increasing x and it turns cubic for x > 0.3. All these structural and ferroelectric properties change due to change in the c/a ratio. Temperature dependent Phonon spectroscopy results (80-500 K) indicate decrease in tetragonal to cubic phase transition temperature upon x due to reduction in anisotropy. Overdamping of ~90 cm-1 E soft phonon mode and dramatic decrease of the intensity of ~160 cm-1 A-mode were observed around the tetragonal ferroelectric to cubic paraelectric phase (< 300 K). The energy storage density of these thin film capacitors were estimated using the measured polarization hysteresis loops and were compared. For x = 0.7, a larger energy storage density (Ure) ~29 J/cm3 with efficiency of ~48 % was estimated at an applied voltage of 1.1 MV/cm. Nearly room temperature transition temperature Tc, larger dielectric constant and high energy density values of our BST1-x thin film capacitors indicate its possible application in high energy storage devices. These results will be presented in details in the meeting.

Abstract ID: 819
Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)
Invited Talk
Topics: Materials Integration
Keywords: Graphene, Copper, Electroless Plating

Graphene aided green electroless copper plating via light/defect structure-triggering

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Copper is known for its high electrical conductivity, malleability and corrosion resistance. These properties make copper a popular choice for coating components in a wide range of industries — from aerospace and automotive to electronics and telecommunications. Many industries rely on copper electroplating for their electrical, industrial, and heating applications due to the material's conductivity and thermal properties. Copper electroplating can also be used as an undercoat before applying other coatings or as a treatment for surfaces before soldering. In electronic industry, copper plating and deposition are essential. Printed circuit board manufacturing and integrated circuit fabrication requires copper plating or deposition.

Generally, in electroless copper (Cu) plating, formaldehyde is used as a reducing agent in coating bath which also consists Cu ions, stabilizer, complexing agent and additives. However, in view of the biological toxicity of formaldehyde, development of environment friendly reducing agent is critical. In this work, an electroless Cu plating is developed through light-triggering reduction reaction occurring on the surface of graphene/Cu foil in the presence of Cu ions. The ultra-thin cuprous oxide (Cu2O) detected by Tip-enhanced Raman Spectroscopy (TERS) provides the hot electrons under resonant light irradiation. The generated hot electrons are concentrated on the defect site of graphene. Comparing to hexagonal structure, the defect site with abundant electrons and lower work function triggers the reduction of Cu, as evidenced by the in situ Raman spectroscopy and X-ray photoelectron spectroscopy (XPS), which demonstrates that the initial Cu reduction reaction is localized at the defect site and forms strong interaction. Under prolonged resonant light irradiation, the reduction reaction continues along the edges of the reduced Cu nanoparticles until they are connected to each other and cover the entire surface of the graphene. Consequently, the resulting coating layer has even better electrical and thermal conductivities since these conductivities are superior for graphene in comparison to copper itself. This developed reduction methodology shows high potential in the applications of high-density integration, catalysis and Cu wastewater treatment.

Abstract ID: 820

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: functional materials, nanostructured semiconductors, gas sensing

Nanosized semiconductors as functional materials for gas sensing

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The great expectations of the gas-sensor market have fostered research in material science and technology toward constant development. In particular, the search for materials should accomplish high sensitivity and low-power consumption. In the last years, a wide plethora of sensing materials has been developed, from traditional (e.g. ceramic thin/thick films) to nanostructured (e.g. nanowires, nanosheets, nanoflowers) semiconductors, including novel low-dimensional semiconductors (e.g. graphene, black phosphorus, metal organic frameworks).

The great challenge of low-dimensional nanostructured materials lies in the control of their properties by the morphology and the grain size, which combines bulk and surface effects. One-dimensional nanostructures are ideal for investigating the dependence of electrical transport, mechanical and optical properties on size and dimensionality. Two-dimensional nanostructures are ideal components for nanoscale devices, due to their high surface-to-volume ratio, fascinating photocatalytic and optical activities.

Most common conventional gas sensors are based on three-dimensional Metal Oxides (MOX). These devices are low-cost and provide high sensitivity, but they suffer of poor stability over the time and need high power consumption to heat up the transducer for recovery, which restricts their use in portable sensing systems. The performance of MOX-based sensors depends crucially on their dimensions, morphology, composition, and surface activity. Among the several parameters that influence the sensing properties of a MOX sensor, the potential barrier at the interface between grains is a major physical quantity. In this sense, the broad assortment of one-, two- and three-dimensional MOX nanostructures has been a precious source for gas sensors technology, which owes its constant development to the requirements of physical, chemical and biological detection systems.

Abstract ID: 821

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Superabsorbent polymer, Guar gum, Hygiene product, Swelling, Environment

Synthesis and characterization of a new highly absorbent material based on carboxymethyl guar gum as an alternative to conventional absorbents in disposable hygiene products

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Superabsorbent polymers (SAPs) are cross-linked networks of hydrophilic polymers with a high absorption capacity of water and aqueous solutions. They have attracted a lot of attention due to their exceptional properties. This has made them ideal for a wide range of valuable applications in medicine, agriculture, and industry in general. However, their greatest application is as a liquid-absorbent material in disposable hygiene products. Disposable baby diapers, feminine sanitary napkins, and incontinence protection for the personal care market are rapidly improving. This market is growing rapidly in regions with very high birth rates and aging demographics, such as developing countries, where superabsorbent materials are among the materials most in daily demand in the market. These days, most commercially available superabsorbent products are made from petroleum-based vinyl monomers, therefore, they are not biodegradable and environmentally friendly. In response to this challenge, environmental protection laws are beginning to encourage the use of renewable and biodegradable materials because of their low production cost and biodegradability. In this context, superabsorbent polymers of natural origin derived from polypeptides and polysaccharides have undergone chemical and biochemical modifications to improve their ability to absorb and retain large quantities of liquids.

The objective of this research is to develop a new highly absorbent material capable of absorbing a large amount of water, based on a guar gum chemically modified and reinforced with a mineral charge. The chemical structure of the material has been characterized by Fourier Transform Infrared Spectroscopy (FTIR), Thermogravimetric Analysis (TGA/DTA), Scanning Electron Microscopy (SEM), and X-ray Diffraction (XRD). The swelling performance of the new material was also investigated. The centrifuge retention capacity (CRC) is about 30 g/g and the absorbency under load (AUL 0.3 psi) is not inferior to 14 g/g in saline solution (0.9 % w/w). Furthermore, a comparison of the swelling capacities of the synthesized material with commercial SAPs extracted from hygiene products showed that the performance was somewhat similar, which favors the use of this natural-based material.

Abstract ID: 822

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Anodes and cathodes Materials
Keywords: Silicon Clathrates, Li-ion Battery Anodes, Li Insertion, Li Migration

Structural Origin of Reversible Li Insertion in Guest-Free, Type-II Silicon Clathrates for Applications as Li-ion Battery Anodes

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The guest-free, type-II Si clathrate (Si136) is an open cage polymorph of Si with structural features amenable to electrochemical Li storage. However, the detailed mechanism for reversible Li insertion and migration within the vacant cages of Si136 is not established. Herein, X-ray characterization and density functional theory (DFT) calculations are used to understand the structural origin of electrochemical Li insertion into the type-II clathrate structure. At low Li content, instead of alloying with Si, topotactic Li insertion into the empty cages occurs at ≈ 0.3 V versus Li/Li+ with a capacity of ≈ 231 mAh g−1 (corresponding to composition Li32Si136). A synchrotron powder X-ray diffraction analysis of electrodes after lithiation shows evidence of Li occupation within the Si20 and Si28 cages and a volume expansion of 0.22%, which is corroborated by DFT calculations. Nudged elastic band calculations suggest a low barrier (0.2 eV) for Li migration through interconnected Si28 cages, whereas there is a higher barrier for Li migration into Si20 cages (2.0 eV). However, if Li is present in a neighboring cage, a cooperative migration pathway with a barrier of 0.65 eV is possible. The results show that the type-II Si clathrate displays unique electrochemical properties for potential applications as Li-ion battery anodes.

Abstract ID: 823

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Electrode/electrolyte interface phenomena

Keywords: Graphene, Au Anodes, SEI, Li-Ion Battery, Mechanical Behavior

Touching the forming SEI layer on Li-ion battery anodes

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The successful transition towards electromobility on the ground and in the air alike requires ongoing improvements in the performance of rechargeable battery systems. One bottleneck for state-of-the-art lithium-ion batteries is controlling the so-called solid electrolyte interphase (SEI) which is key for ultimately advancing the life-time of lithium-ion batteries, for obtaining higher rates, and arrive at an increased safety. Interfaces are essential in electrochemical processes, providing a critical nanoscopic design feature for composite electrodes used in Li-ion batteries. Understanding the structure, wetting and mobility at nano-confined interfaces is important for improving the efficiency and lifetime of electrochemical devices. For Si and Si-composite materials used as anodes the interfaces still pose a major issue. Employing additives and using for characterization an electrochemical surface force apparatus, atomic force microscopy, and (hard) X-ray photoelectron spectroscopy it is possible to control the growth and to investigate the mechanical properties of an SEI in a lithium-ion battery

environment. With a new approach of an electrochemical “battery” SFA we present first studies on a gold model system1,2 and graphene3 anodes. The force behavior reveals a compressible film at all stages of SEI growth3 and can be used to study wetting phenomena2 in confined geometries. The demonstrated methodology provides a unique tool for analyzing electrochemical battery interfaces, in particular in view of alternative electrolyte formulations and artificial interfaces.

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Abstract ID: 824

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Theory of graphene, Mxenes and other two-dimensional materials

Keywords: Graphene, Quantum dots, Optical Properties, Defects

Theory of electronic and optical properties of pristine and defective graphene quantum dots

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Graphene quantum dots (GQDs) are 0D carbon-based materials that exhibit several striking characteristics of graphene combined with a tunable bandgap due to quantum confinement effects. The tailoring of the optical bandgap of GQDs can be achieved by varying their shape, size and also by introducing topological anomalies like Stone-Wales (SW) defects. In order to realize the full potential of pristine and defective graphene nanostructures in optoelectronic applications, it is essential to obtain a deep understanding of their electronic structure and optical properties. In this talk, we will discuss the theory of electronic structure and optical properties of these GQDs, within a Pariser-Parr-Pople (PPP) model Hamiltonian-based correlated electron approach, developed in our group. We will present results of theoretical calculations of the optical absorption spectra of pristine as well defective GQDs of different shapes and sizes. Our calculations have revealed that the absorption spectra are redshifted with the increasing sizes of quantum dots. Our studies also demonstrate that SW type reconstruction is responsible for the appearance of new defect-induced peaks below the optical gap and dramatically modifies the optical absorption profile. In addition, our investigations signify that electron correlation effects become more dominant for SW-defected GQDs. We finally establish that the introduction of SW defects at specific locations strongly enhances light absorption in the visible range, which is of prime importance for designing light-harvesting, photocatalytic, and optoelectronic devices.

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Abstract ID: 825

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Photocatalytic and electrochemical water splitting
Keywords: Anodized nanotubular arrays, Gas phase photocatalysis, High-purity hydrogen production

Anodized metal oxide nanotubular arrays for gas-phase photocatalysis and photo-induced high-purity hydrogen production

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So far, in order to enhance photocatalytic activity of metal oxide semiconductor materials with wide bandgaps such as hematite (a-Fe2O3) and TiO2, self-aligned nanotubular structures with large specific surface area prepared by electrochemical anodization have been intensely studied due to their attracting features such as simplicity and low cost fabrication. Electrolytes including both fluoride and polyols for anodic metal oxide have been widely employed owing to their better controllability for obtaining different nanostructures. In fact, well-aligned metal oxide nanotubes with smooth walls were produced and those applications toward water photooxidation and air purification with high performance were demonstrated. In this presentation, I will introduce our recent results on visible-light-responsive gas-phase photocatalysis over the anodized hematite nanotubular arrays loaded with platinum or cuprous oxide (Cu2O) nanoparticles. In addition, photo-induced high-purity hydrogen production based on a bilayer membrane of an anodized TiO2 nanotubular array and an electroless-deposited palladium layer will be also presented.

Abstract ID: 826

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanoparticles, Nanowires, and 3D Structures

Keywords: crossed-wire woodpile; antenna effect; hot spot effects; plasmon-enhanced fluorescence (PEF); surface-enhanced Raman scattering (SERS)

Three-dimensional plasmon-generating nanostructure for surface- enhanced Raman scattering and plasmon-enhanced fluorescence detection

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In this study, silver nanowire 3D random crossed-wire woodpile (3D-RCW) nanostructures were designed and prepared. The 3D-RCW provides rich “antenna” and “hot spot” effects that are responsive for surface-enhanced Raman scattering (SERS) effects and plasmon-enhanced fluorescence (PEF). The optimal construction mode for the 3D-RCW, based on the ratio of silver nanowire and control compound R6G, was explored and established for use in PEF and SERS analyses. We found that the RCW nanochip capable of emission and Raman-enhanced detections uses micro levels of analysis volumes. Consequently, and SERS and PEF of pesticides (thiram, carbaryl, paraquat, fipronil) were successfully measured and characterized, and their detection limits were within 5 μM~0.05 μM in 20 μL. We found that the designed 3D plasmon-enhanced platform cannot only collect the SERS of pesticides, but also enhance the fluorescence of a weak emitter (pesticides) by more than 1000-fold via excitation of the surface plasmon resonance, which can be used to extend the range of a fluorescence biosensor. More importantly, solid-state measurement using a 3D-RCW nanoplatform shows promising potential based on its dual applications in creating large SERS and PEF enhancements.

Abstract ID: 827

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: All solid-state batteries

Keywords: Argyrodite, Indentation Size Effect, Microhardness, Dislocation

Changes in the mechanical properties of (Cu1–xAgx)7GeSe5I superionic crystals upon isovalent substitution

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Crystals with an argyrodite structure are promising materials for the production of fuel cells, supercapacitors, and solid-state ionics devices. They have mixed electron/ion conductivity. Ionic conductivity in (Cu1-xAgx)7GeSe5I crystals is realized through unfilled vacancies in the cation sublattice. These materials are characterized by a high structural disorder in the sublattice of mobile ions. Different degrees of structural disordering in these crystals can be achieved by isovalent substitution, in which a number of solid solutions are formed. The changes in the mechanical properties of mixed crystals (Cu1-xAgx)7GeSe5I have not yet been investigated. In this work are presented the results of studies of microhardness for (Cu1-xAgx)7GeSe5I mixed crystals, as well interpretation of microhardness size effects within the framework of the gradient theory of plasticity.

(Cu1-xAgx)7GeSe5I mixed crystals, grown by Bridgman-Stokbarger methods, were used to measure microhardness. Measurements of the microhardness H were carried out at room temperature using PMT-3 microhardness-meter with the Vickers indenter. The microhardness H were determined by using the equation H=18.54*P/d2 where P is load force on the indenter, d is the diagonal of the imprint. Microindentation was performed in the direction of applying force (001). When the load on the indenter changes (0.02 N - 2 N), the dimensional effect of indentation (H(h)≠const) is observed. The dependences H(h) showed two sections with different rates of decrease in hardness with an increase in the indentation depth h. The observed size effects were interpreted in the framework of the theory of Strain Gradient Plasticity. It was shown that at small indentation depths, the main mechanism of plastic deformation of crystals is the motion of statistically distributed dislocations in the microcontact region. The dependences H(h) are well approximated by straight lines in the region of large values of h in the coordinates “H2 - h-1” according to the formula of the gradient theory of plasticity: H/H0=(1+h*/h)0, where H0 and h* are parameters of model of geometrically necessary dislocations. The formation of geometrically necessary dislocations in the region of the microcontact is the mechanism of plastic deformation of crystals in the region of linear approximation of the dependences H(h).

The parameters H0 and h* for (Cu1-xAgx)7GeSe5I mixed crystals were determined. It was found that upon isovalent substitution Cu +⟶ Ag+, the microhardness of (Cu1-xAgx)7 GeSe5I mixed crystals decreases monotonically from 2.7 GPa to 1.1 GPa.

Abstract ID: 828
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Bio-composites
Keywords: Agro-residue; bio-composite; Natural Fibers; Recycled Plastics; Production

Production of Sustainable Bio-Composites from Agro-residue Fibers and Recycled Polypropylene

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Wood Plastic Composites (WPCs) have captured a considerable attention in various applications due to their inherent properties like strength and lightweight over conventional polymers. However, using wood as an organic filler for polymers pose a serious challenge to the green areas. Hence, utilization of agro-residues as fillers instead of wood is one of the sustainable solutions to the aforementioned problem. Also, the exploitation of recycled polymers mainly from Municipal Solid Waste (MSW) to produce value added products with economic edge will overcome the adverse impact of polymer waste on the environment. As such, recycling appears to be a valuable future route for sustainable production in polymer-related industries. Thus, research on development of new types of bio-composites prepared using various recycled components is being actively pursued. In this context, our study aims to investigate the potential use of date palm fibers extracted from agro-residue pedicles as a natural filler for synthetic polymers like virgin polypropylene and recycled post-consumer polypropylene. The use of raw and chemically treated fibers is studied and compared. Three levels of fiber content (10 v.%, 20 v.% and 30 v.%) are adopted to manufacture such new class of bio-composites. The influence of date palm fiber content and treatment process on the mechanical and physical performance of the developed bio-composites will be explored. Mechanical testing, hardness, and water absorption of the fabricated specimens are conducted in accordance with ASTM standards. Fourier Transform Infrared Spectroscopy (FT-IR), X-ray Diffraction (XRD), Thermo-Gravimetric Analysis (TGA), and Differential Scanning Calorimeter (DSC) tests are also performed.

Abstract ID: 829

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanomaterials and Nanotechnology

Keywords: Surface plasmon – exciton coupling, Plexcitons, Thermoresponsive hybrid nanosystem, Photoluminescence

Temperature driven plasmon-exciton coupling in thermoresponsive dextran-graft-PNIPAM / Au nanoparticles / CdTe quantum dots hybrid nanosystem

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The temperature driven plasmon-exciton coupling in thermoresponsive dextran-graft-PNIPAM / Au nanoparticles / CdTe quantum dots (D-g-PNIPAM / Au NPs / CdTe QDs) hybrid nanosystem was studied. A significant (0.84 eV) splitting of the absorption peak was observed in the absorption spectrum of the nanosystem, which reflects the fact of formation of plexcitons, occurring due to strong plasmon-exciton coupling. An increasing with time plasmonic enhancement of the photoluminescence of CdTe QDs was revealed, as a result of the penetration of quantum dots into the volume of the D-g-PNIPAM / Au NPs hybrid nanosystem and bonding to it. The heating-cooling cycle of the aqueous solution of the studied nanosystem leads to a reversible quenching-recovery alteration of the QD photoluminescence. The quenching was rationalized as a result of an increased probability of nonradiative resonance energy transfer (RET) from CdTe QDs to Au NPs, which occurs due to shortening of the NP-QD distance, caused by shrinking of the macromolecule due to cooling-induced lower critical solution temperature phase transition. Increasing the NP-QD distance in the heating stage recovers the QD PL intensity. The observed effect opens up opportunities for the controlled reversible temperature-driven tuning of the photoluminescence intensity of D-g-PNIPAM / Au NPs / CdTe QDs nanosystem, which is highly important for its potential use in photonics and biomedical applications.

Abstract ID: 830
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Bio-composites
Keywords: Bio-composites, Natural fillers, Natural Waxes, Fiber/Matrix Adhesion

PLA- and PHBV-based Bio-composites: Improvement of the Mechanical Properties by Fiber Surface Treatment with Natural Waxes

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Thermal, mechanical and viscoelastic properties of bio-composites of poly(lactic acid) (PLA) and poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) with natural fibers (bran and potato pulp powder), untreated and treated with natural waxes (carnauba and bee waxes), were investigated.

The aim of the study was to verify a potential valorization of agri-food by-products and, in addition, to reduce the final cost of PLA- and PHBV-based materials.

The results showed that untreated bran fibers and potato pulp powder acted as fillers, and not as reinforcement, for PLA and PHBV, due to poor fiber/matrix adhesion, because a small loss in mechanical properties (tensile strength and elongation at break) was detected.

To try to improve the mechanical response, surface treatment of the natural fibers with carnauba and bee waxes was performed. This procedure was found to improve the properties of the bio-composites, enhancing the biopolymer/fiber adhesion, as confirmed also by predictive theoretical models. In addition, the presence of natural fibers promoted biodegradation and in particular the disintegration of the bio-composites in compost.

Thus, the addition of bran fibers and potato pulp powder, treated with natural waxes, turned out to be a method useful (i) to valorize abundant agri-food by-products, according to circular economy principles, and (ii) to reduce the final cost of PLA- and PHBV-based materials.

Key Words: Bio-composites, Natural fillers, Natural Waxes, Fiber/Matrix Adhesion

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Abstract ID: 831

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: 3D printing, ceramic matrix composite

Effects of Reinforcements on 3D Printed Polymer-Derived SiOC

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Ceramic matrix composites (CMCs) are a class of structural material that are used in propulsion systems, hypersonics and nuclear power processing plants. Due to their ceramic matrix, CMCs exhibit high temperature stability at light weight (compared to metals). The reinforcements, usually in the form of fibers, particles or platelets, increase the strength and toughness of CMCs. HRL has developed a new manufacturing method that fabricates CMCs via 3D printing of reinforced polymer-derived ceramic. Using a matrix of silicon oxycarbide (SiOC) reinforced with mullite particles, we demonstrated an increase in fracture toughness from 1 MPa m1/2 in the neat material to >3 MPa m1/2 in the reinforced material. Further, we investigated the effects of an array of ceramic reinforcements, including mullite, Al2O3, silicon nitride (Si3N4), and silicon carbide whiskers, ranging from 0-40% by volume.

Abstract ID: 832
Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)
Invited Talk
Topics: Nanomaterials and Nanotechnology
Keywords: Nano, Materials, Band Alignment, Contacts, Spin

Atomically Precise Chemical, Physical, Electronic, and Spin Contacts

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Two seemingly conflicting trends in nanoscience and nanotechnology are our increasing ability to reach the limits of atomically precise structures and our growing understanding of the importance of heterogeneity in the structure and function of molecules and nanoscale assemblies [1]. By having developed the “eyes” to see, to record spectra, and to measure function at the nanoscale, we have been able to fabricate structures with precision as well as to understand the important and intrinsic heterogeneity of function found in these assemblies. The physical, electronic, mechanical, and chemical connections that materials make to one another and to the outside world are critical and are intertwined in terms of their function. Just as the properties and applications of conventional semiconductor devices depend on these contacts, so do nanomaterials, many nanoscale measurements, and devices of the future. We discuss the important roles that these contacts can play in preserving key transport and other properties. Initial nanoscale connections and measurements guide the path to future opportunities and challenges ahead. Band alignment and minimally disruptive connections are both targets and can be characterized in both experiment and theory [2]. Chiral assemblies can control the spin properties and thus transport at interfaces [3]. I discuss our initial forays into these areas in a number of materials systems.

Key Words: Nano, Materials, Band Alignment, Contacts, Spin

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Abstract ID: 833

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Fuel Cells

Keywords: CGO, LSCF, pore-former, cathode, SOFC

Impregnation of CGO-backbone cathodes modified by addition of pore-formers for SOFC application.

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Impregnation of CGO-backbone cathodes modified by addition of pore-formers for SOFC application.

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Solid oxide fuel cells (SOFCs) are promising devices for energy-conversion applications due to their high electrical efficiency and eco-friendly behavior [1-2]. Their performance is not only influenced by the microstructural and electrical properties of the different layers of the unit cell, i.e. electrodes and electrolyte [3]. Indeed it also depends on the interactions at the cathode-electrolyte and anode-electrolyte interfaces [3-4]. Nowadays, commercial SOFCs are electrically efficient at high operating temperatures, typically between 800 and 1000 °C. This high-temperature range restricts their real-life applications, but also their lifetime. Our basic goal deals with the objectives to reduce the operating temperature by working in the range from 500 to 700 °C, and to develop low-cost IT-SOFCs. In the present work, we have elaborated metal-supported solid oxide fuel cells (MS-IT-SOFCs) that would provide very cheap SOFC cells with increased lifetime and reduced operating temperature.

This part of our work focuses on the physical, chemical and electrical characterizations of porous CGO-backbone cathodes which have been impregnated with a LSCF sol-gel solution. The porosity of the backbone was controlled by the addition of different pore-formers. The performance of 4 different samples was compared by studying the evolution of the electrical resistivity in function of temperature. We have demonstrated an important effect: whatever the temperature, from 500 to 700 °C, the cathode resistivity can be tuned both by the LSCF solution viscosity and by the kind of pore-former.

Key Words: CGO, LSCF, pore-former, oxide, cathode, SOFC.

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Abstract ID: 834

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Graphene, THz, Ultrafast modulation

Ultrafast control in THz graphene-based metasurfaces

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We discuss the unique possibilities stemming from exploiting the exotic properties of artificial metasurfaces designed for operation in the THz regime. Metasurfaces are electromagnetically ultrathin artificial materials with macroscopic properties defined by the architecture of the building blocks, the meta-atoms. Adjusting the meta-atoms enables the control over different aspects the electromagnetic waves and the realization of unusual electromagnetic functions. Within this framework we present various groups of metasurface configurations incorporating different constituent materials. We mainly focus on graphene based metasurfaces acting as modulators for the THz regime. Graphene, the acclaimed two-dimensional (2D) material made of carbon atoms arranged in a honeycomb lattice, exhibits unique optical properties particularly in the THz spectrum, where it predominantly exhibits a Drude-like response. Here we present that ultrafast modulation response in a graphene thin film absorber which can be assessed with use of a broadband THz time-domain-spectroscopic system (THz-TDS) in an IR pump-THz probe configuration. The simple structure consisting of a graphene sheet is placed over a back platted dielectric substrate, forming an electromagnetic cavity. The cavity provides the means for achieving critical coupling and hence increased tunable absorption. The near-IR stimulus generates hot carriers in the graphene metasurface which effectively reduces its THz conductivity. Similar phenomenon can be induced by self-modulation using intense THz fields. The simple scheme of the absorber can be used as a platform for ultrafast flat optics and metasurfaces. Apart from that, we review additional recent THz metasurface findings with some interesting features. For example it has been shown, that using the IR pump-THz probe configuration in hybrid metasurfaces with metals combined with photo-conducting semiconductors one is able to produce switchable and tunable terahertz electromagnetic functions.

Abstract ID: 835
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Polymeric composites
Keywords: Cellulose nanocrystals; Pickering emulsion; Double emulsion; Capsule

Hybrid materials obtained from the polymerization of Pickering emulsions stabilized by cellulose nanocrystals

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Cellulose nanocrystals (CNC) are biorenewable particles of rising interest for the stabilization of Pickering emulsions. They are commonly extracted from cellulose substrates, and are needle-shaped nanoparticles (150-200 nm in length, 5-20 nm in width)1. In the present work, direct, inverted and double emulsions were stabilized using surface modified CNC. Brominated functions grafted bring wettability to the CNC allowing its adsorption at different water/oil interfaces. Taking advantage of this modification, the stabilized emulsions were further polymerized by whether free or controlled radical polymerization leading to objects with a very broad range of morphologies depending on the polymerized phase and initiation locus. The focus was brought on inverse emulsions because very little study was conducted on such systems2, as they require modification of the CNC. Solid foams were obtained3 when the polymerization was conducted into the continuous phase while suspension polymerizations of water-in-oil emulsions lead to either full beads or empty capsules. Likewise, elaboration of a new type of capsules (hollow/porous microcapsules) was investigated, by using double emulsions as template and polymerizing their intermediate phase.

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Abstract ID: 836

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Stability of Nano, Micro and Macro Composite Structures

Keywords: TiAlN, selective absorber, nanophotonic, broadband absorbers, stability, magnetron sputtering

Growth of robustly stabile nanophotonic structures by a viable technique: blackbody absorbers

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Growing efficient blackbody character absorbers by a simple method, has proven to be challenging for various applications such as solar energy, thermal regulation and suppression of stray light for the optical devices. Nanostructured refractory materials afford exceptional features to manipulate incident photons of light at subwavelength scale and withstand against severe conditions. Here, we report a sputtering technique-based method to produce TiAlN black absorbing coatings with vertically aligned columnar nanostructure, as a unique approach to produce large area metamaterials. The fabrication process is simple, free of any sophisticated patterning approach, substrate-independent (conducting, insulating, single crystal, amorphous, rigid or flexible), viable and capable to easily be up scaled, benefitting excellent adhesion and appropriate corrosion resistance of the absorbing coatings. An average absorptivity, □ = 0.89, covering a broad range of wavelengths, 200 nm to 2500 nm, was achieved from the single nanostructured coating and increased to □ = 0.95 after grading with thin anti-reflecting layers, which is higher than any other PVD deposited ceramic coatings on smooth substrates. Robust stability in adverse environments is an exceptional feature of our broadband super absorbers. The proposed sputtering based fabrication process would open new platform to design, prepare and integrate nanophotonic structures.

Abstract ID: 837
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Bio-composites
Keywords: calcium alginate, graphene, biotin, pyrrole, TiO2, bioluminescence

Functional tailored soft nanobiocomposites of hybrid hydrogel-derived composite materials

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Our laboratory has used calcium alginate hydrogels as a preferred medium to create tailored nano-bio-composite hybrid functional materials. Indeed, we use as a base various covalently derived hybrid alginate composites enabling to provide it with varying functional abilities, such as conductivity (alginate-pyrrole (poly) (1)), affinity (biotin-alginate) (2), resin (alginate-amino acid). These were used for various applications, including optical and electrochemical biosensors (3), cell-base biosensors or bioremediation (5). One useful feature of our system is that we can mix these composites between themselves providing mixed functionalities such as alginate-pyrrole with alginate-biotin (6). In addition this hydrogel enables to entrap various types of materials such as graphene (7), TiO2, bioluminescent bioreporter whole bacterial cells, and so on. We describe, herein, the physical and chemical versatile properties of a hydrogel which has the unique capability to produce self-assembled interpenetrated porous tailored functional polymers, be they single, or multiple, and in addition, enabling to entrap within itself inorganic materials or even living biomass, such as cells. Another important feature of this system is that it can be used in 3D printing, opening up to a promising future. And finally, the three-dimensional features that are simply obtained by the addition of calcium enabling reticulation, can be simply reversed via phosphate or other chelating agent.

Key Words: calcium alginate, biosensors, graphene, TiO2, biotin, pyrrole

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Abstract ID: 838

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Functional Magnetic Materials

Keywords: MgB2 superconductor, superconductor Bi2Sr2Ca2Cu3O10, NdFeB permanent magnet recycling, Spark Plasma Sintering, Texturing

Overview of spark plasma sintering of functional ceramics

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Abstract: The non-conventional Spark Plasma Sintering (SPS) process is based on the combination of a high current and a mechanical high pressure applied directly to the powder material. This technique presents the advantage to provide the possibility to obtain dense materials in a few minutes while mastering their microstructure. A lot of works have been reported since the introduction of SPS in research laboratories, and many groups have tried to understand the densification mechanisms involved.

After a brief history of the SPS technique, the characteristics of this process will be detailed and compared to those of the other sintering techniques.

On the other hand, the densification, the texturation and also the functionnal properties of materials sintered by SPS will be discussed. We'll successively consider: i) the sintering of recycled Nd2Fe14B magnets; ii) the fabrication of superconducting MgB2 cryo-magnets and iii) the fabrication of layered superconducting Bi2Sr2Ca2Cu3O10 bulks. In this last case, the SPS equipment was modified in order to obtain textured bulk samples. This new process is referred to as "Spark Plasma Texturing" (SPT). During SPT, the bulk material can freely deform. As a result, a preferential crystallographic orientation of the grains is obtained. The anisotropic properties resulting from the grain alignment will be discussed.

Abstract ID: 839

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Correlated Electrons

Keywords: Synthesis; Bis-imidazole Stokes shift; Probe; CMC.

Synthesis and Physicochemical investigation of novel bis-imidazole derivative

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Pyrene based bis-imidazole 4,4',5,5'-tetraphenyl-2,2'-di(pyren-1-yl)-2'H-1,2'-biimidazole (PY-BISIM) was synthesized by ferricyanide oxidation of 4,5-diphenyl-2-(pyren-1-yl)-1H-imidazole. PY-IM was synthesized by the reaction of pyrene-1-carboxaldehyde with benzil in the presence of ammonium acetate in acetic acid. The structure of the PY-BISIM was confirmed by the IR, 1H-NMR, 13C-NMR and Mass spectra analysis. Absorption and emission spectrum of the PY-BISIM has recorded by using ten different solvents and as polarity increases, the absorption and emission showed bathochromic shift. Different physicochemical properties such asmolar absorptivity, stokes shift, oscillator strength, transition dipole momentand fluorescence quantum yield of newly synthesized PY-BISIM has been studies in different solvents. In addition effects of two surfactants certyltrimethyl ammonium bromide (CTAB) and sodium dodecyl sulfate (SDS) on emission spectrum of PY-BISIM has been studied and findPY-BISIM can be used as probe or quencher to determine the critical micelle concentration (CMC) of the CTAB and SDS surfactants.

Abstract ID: 840

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: 2D MOF, coordination polymers, hydrophobic nano-sheets

Permethylated two-dimensional Metal-Organic Frameworks - Promising Candidates for Emerging 2D Materials

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After the discovery of graphene with the set of properties that essentially distinguish it from other carbon allotropes, ultra-thin layered materials, classified as 2D nanomaterials, enjoy growing interest due to their unique properties [1]. In this context, although three-dimensional metal-organic frameworks (3D MOFs) are currently studied for addressing challenges concerning energy and environment, recently two-dimensional MOFs have become of interest from the perspective of their approach as 2D materials. The possibilities of variation of their construction units (metal and ligand) allow the fine control of the material properties. But during the forming process, the 2D layers are stacked by intermolecular interactions, leading to materials with increased dimensions. To study specific properties of 2D material, it must be delaminated and isolated as individual layers with a thickness/surface ratio as small as possible, which is a challenge. Both the top-down and bottom-up approached strategies proved to be quite difficult involving large consumption of time, materials, energy, etc., without guaranteeing the stability of the individual layers.

A promising alternative pathway is the design and synthesis based on suitable precursors of two-dimensional metal-organic networks with extremely weak intermolecular interactions, which facilitate delamination in nanosheets [2,3]. Our original approach consists in the use of ligands containing permethylated silicone units, which by their natural exposure and low surface tension shield the 2D structure and prevent the establishment of quantifiable interactions among neighboring layers. Binary mixtures of ligands with a dicarboxylic acid with tetramethyldisiloxane spacer and different bipyridyl derivatives for different metal ions (Co, Zn, Mn, Cd) were used successfully. The obtained structures were evaluated in terms of structure, size, morphology and properties (thermal, magnetic, electrical, optical). Preliminary assessments have been made regarding the ability to respond to external stimuli. Acknowledgements: This work was supported by a grant of Ministry of Research and Innovation, CNCS - UEFISCDI, project number PN-III-P4-ID-PCE-2020-2000 (2D-PerMONSil), within PNCDI III, Contract 207/2021.

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Abstract ID: 841

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Nanobiosensor technology, Real-time crop health monitoring, Phytodiagnostics, Smart Agriculture, Electronic devices actuators

Nanosensors Technology: Recent Advances for Smart Intelligent Agriculture

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Nanobiosensors can play an important role in revolutionizing the agriculture through the development of next generation diagnostic tools and techniques. Various types of nanobiosensors have been reported for detection and monitoring plant signal molecules and metabolic contents related with biotic and abiotic stresses. Nanobiosensors have unprecedented levels of performance for sensing ultra-trace amount of various analytes for in vivo measurement. These nanobiosensors communicate with and actuate electronic devices for agricultural automation. Thus, both biotic and abiotic plant stresses and nutritional deficiency are monitored in real-time to report crop health status for precise and efficient use of resources. Recently, there has been a remarkable growth in the development of a wide range of nanosensors including fluorescence resonance energy transfer-based nanosensors. These nano-sensors and nano-based system have some unique characteristics such as small size, portable, efficient, specific, sensitive and relatively inexpensive. Engineered nanomaterials in nanobiosensors can be embedded in plants for monitoring signaling molecules by various communication techniques. Nanosensors communicate with and actuate electronic devices for improving crop productivity by optimization and automation of water and agrochemical allocation. So, they can prove to be a very effective tool for smart delivery systems, promoting soil health, crop protection and disease management.

Fundamentals and development in nanosensor technology for sensing in smart agriculture and how nanosensors in plants can communicate with and actuate electronic devices for optimizing crop growth and yield in response to resource scarcity or stresses by collecting real-time data about the crops, soil and surrounding conditions through wireless sensor networking technology will be addressed in the presentation. The presentation will also offer updated information collected from state-of-the-art reviews and research articles on smart nanosensor technology in agriculture including wearable devices, wireless nanosensors networks, real-time crop health status, monitoring plant diagnostics using signaling molecules, nanosensor communications and actuation of electronic devices. Hence, the recent advances in nanosensors technology and their applications for smart intelligent agriculture will be discussed in the presentation.

Key Words: Nanobiosensor technology, Real-time crop health monitoring, Phytodiagnostics, Smart Agriculture, Electronic devices actuators

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Abstract ID: 842
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Porous and cellular materials
Keywords: nanoporous, hierarchical, 3D, self-power, water oxidation, water purification

Structural Design and Manufacturing of Three-Dimensional Porous Superstructures with Additive and Subtractive Electrochemistry for Flexible Self-Powered Electronics, Nanoelectromechanical Devices, and Water Purification

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The recent search for advanced materials with desired properties for the next-generation flexible energy devices, electronics, and environmental remediation has been focused on the unique class of three-dimensional (3D) porous superstructures that can be made of myriad materials and their composites, including 2D materials, metals, oxides, and polymers.

Herein, we report an original and rational scheme to create 3D metallic foams with tunable multi-level porosity by using a process consisting of additive electrodeposition and subtractive electroetching. The resulted metallic foams can readily serve as catalytic templates for the growth of 3D free-standing hierarchically porous thin graphite and metal-alloy-oxide composites that offer enhanced mechanical, electric, catalytic, and electrochemical performances. The feature size and morphology of the porous structure can be readily tuned and predictably fabricated with Gaussian-regression-based machine learning. The obtained materials have integrated as the flexible energy units in self-powered strain sensors and nanomotor manipulation systems, and applied for catalysis of water oxidation and water purification.

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Abstract ID: 843
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Polymeric composites
Keywords: Key Words: nano, composite, silicone, superhydrophobicity

Superantiwetting Polymeric Nanocomposite Materials: From Coating to Bulk Material

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Wetting and antiwetting is an important property of solid materials no matter if it is required or annoying. Several technologies have been reported to prevent wetting by water, oil, or even both. A major contribution was the development of silicone nanofilaments (SNFs) leading to extreme antiwetting coatings and meanwhile used in the industrial world. SNF technology is based on the new Droplet Assisted Growth and Shaping (DAGS) synthesis approach where the formation of water nanodroplets is the key step for defining the shape of nanostructures finally providing superantiwetting properties to a surface. Beside this, we will demonstrate a further step, how these materials can be further improved by nanocomposite approaches and we will introduce a tremendous step forward to stable superhydrophobic bulk polymer materials which do not suffer from the vulnerability of coatings. We will show a fluorine-free superhydrophobic bulk material with mechanochemical robustness and self-cleaning functionality based on polypropylene (PP) that simultaneously possess mechanochemical robustness and good resistance to oil fouling.

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Abstract ID: 845
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Recycling and sustainability of composite materials
Keywords: Promising cutting tool, Polymer materials, HSS

Prospects for creating tools for disposal of polymer materials with interchangeable cutting plates

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Aerospace manufacturing requires materials that can withstand the stresses encountered in flight while still having a low specific gravity. For this purpose, various composite materials are currently widely used, of which polymeric materials constitute a significant part. Therefore, it will require the development of new methods and tools.

A set of methods was found for the disposal of polymer materials. All of them require pretreatment of polymeric materials, which consists in grinding these materials. Thus, firstly, we need to create more efficient equipment and tools for grinding polymer materials. For example impact crushers HNS400-1000. They are currently a good solution to the problems of recycling and disposal of polymer materials. These installations use special cutting tools.

Currently, knives for knife crushers are made of solid materials from solid materials T41901. This solution has disadvantages associated with the high cost and durability of the knife. To increase the productivity of the knife described above, the new knife is being developed with the replacement of tool steel by high-speed steel. But the main distinguishing feature of the new knife is its geometric configuration, which makes it possible to more than double the resource of the tool and significantly save the material used for its manufacture.

The increase in the resource of the tool occurs due to the fact that in case of wear of the cutting edge of the tool, it can be removed from the knife body, turned 180 degrees, and reinstalled. The material is saved by reducing the size of the plate. The plate is fixed to the knife body with countersunk screws.

The promising cutting tool using the high speed steel indexable insert has advantages. For its implementation, it is necessary to carry out strength calculations under various conditions of loading the cutting part of the tool. It is also necessary to calculate the optimal number of screw connections, their size and location.

Let's make a calculation in the SolidWorks environment by simulating the load on the product. To do this, we will create a 3D model and assemble a promising cutting tool using a replaceable HSS insert.

Set the boundary conditions. Since the knife is attached to the rotor of the machine with bolts, we fix the part in the place where the bolts are fastened. And set the load along the edge of the knife. Let's break it down into a set of finite elements.

It is noticeable that the joints of the knife body and the plate, the screws have a minimum load to ensure the connection. The stress on the promising cutting tool is less than the allowable tensile stress.

Conclusion:

Promising cutting tools for recycling PCM using a replaceable high speed steel insert is suitable for the HNS400-1000 machine.

The development of a promising cutting tool with the ability to reverse the insert is a promising direction for further scientific work, for which it is necessary to carry out calculations showing its effectiveness.

Abstract ID: 846

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Cell fabrication and failure analysis

Keywords: Liquid Phase Transmission Electron Microscopy, in-situ, MEMS, heating, biasing, Electrochemistry, Material Science, Life Science

In-situ Liquid Phase Electron Microscopy: A promising route for Material Science, Energy Storage & Life Science applications

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We introduce a system for in-situ liquid phase studies inside the Transmission Electron Microscope (LPTEM), referred to as the "Stream" System. The latter uses a Micro Electro-Mechanical System (MEMS)-based device as a smart sample carrier, which contains an integrated set of biasing electrodes to enable in-situ electrochemistry, or an integrated microheater to allow liquid heating experiments. As a result, the system provides users with the capability to visualize exciting dynamics in liquid environments as a function of different stimuli. This opens up several possibilities in material science, energy storage and life science applications. Historically, the LPTEM community has been facing several challenges, including uncontrolled liquid layers that affect the imaging resolution and hinder analytical techniques such as electron diffraction, EDS or EELS. Furthermore, controlling the microfluidic environment around the sample (i.e. pressure, flow rate) has proven to be extremely challenging. In order to provide meaningful results and address these historical challenges, our MEMS device controls the flow direction and ensures the liquid will always pass through the region of interest. As a result, the system offers the opportunity to define the mass transport and control the kinetics of the reaction. Furthermore, the system allows to control the liquid thickness well below the beam broadening threshold, enabling resolutions that can go even down to 2.15 Å (for a 100nm liquid thickness). Such control of the liquid thickness enables elemental mapping, allowing users to distinguish the spatial distribution of different elements in liquid. We believe that our development will play a fundamental role in addressing many of the research questions within battery optimization, fuel cells and (electro)catalysis. Furthermore, it will provide unique insights into the chemistry that governs the structure-property relationship of materials, as well as the unique possibility to visualize biological processes in real time with extreme resolutions, without the need of vitrifying the biological specimen.

Abstract ID: 847

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanoparticles, Nanowires, and 3D Structures

Keywords: quantum dot/rod, two-photon fluorescence, electric field, voltage sensing

Quantum dots for two-photon cell transmembrane electric field imaging

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Semiconductor nanoparticles (NPs), more commonly known as quantum dots (QDs) or quantum rods (QRs), exhibit an electric field (E-field) sensitive fluorescence and have been proposed as promising probes for imaging membrane voltages in living cells[1]. Researchers have worked extensively on characterizing the E-field sensitivity of the single-photon fluorescence (1PF) of NPs with a variety of shapes, sizes, and material compositions[2]. And only recently, changes in the fluorescence of membrane-embedded NPs in response to membrane voltages were published[3,4]. In this work, we show that the E-field sensitivity of the two-photon fluorescence (2PF) of type-I and quasi-type-II NPs is more than double with respect to 1PF. Moreover, we have characterized the fluorescence changes in response to transient fields comparable in strength with transmembrane fields in a living cell. Under fast E-field switching, we observe an OFF-transient causing a significant reduction of the fluorescence response to the external E-field, even at frequencies as low as 1 Hz. This severely limits the anticipated performance for the detection of neuronal action. For cardiac electrical activity, however, the impact is limited, and we show that our quasi-type-II QDs can detect a simplified action potential train with an efficiency of roughly 15 % / 60 mV (assuming a 4 nm membrane). These results demonstrate the potential of using QDs/QRs for two-photon action potential imaging in cardiomyocytes.

Figure 1. A) Percentual decrease of the 1PF of 9 nm CdSe/CdS QDs in response to a 400 kV/cm E-field. B) Optical response of the 1PF (top) and 2PF (bottom) to a simulated 30 bpm cardiac action potential train with a ON-level of -150 kV/cm and an OFF-level of 0 kV/cm.

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Abstract ID: 848

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: PV system, MPPT, Backstepping, Lyapunov

Backstepping Control for photovoltaic system connected to grid through inverter with applying method predictive control

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The purpose of this research project is the development of robust and efficient control and state estimation strategies for controlling the photovoltaic connected to grid system. This work focuses on improving the performance of photovoltaic system, through using the advanced control algorithms namely the Backstepping controller for DC / AC power interface control. This control of the DC / AC converter allows to inject a sinusoidal output current synchronized to the network and to improve the quality of energy injected into the network by improving the rise time, the settling time and the steady-state error. A regression plan will be formulated after collecting PV array data from its characteristic curves to provide the reference voltage for tracking the maximum power point (MPP). The asymptotic stability of the system will be proved by using Lyapunov stability criteria. After the system being stable, the method predictive control technique will be applied in the real time inside the controlled in order to anticipate the future behavior of the process. The maximization of the reproduced energy will also be studied using the perturbation and Observation (P & O) logic algorithm. All proposed approaches will be validated by simulation under the Matlab / Simulink environment.

Abstract ID: 849

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Solar Cells

Keywords: 3D Graphene, Alkali Metal Embedded Carbon, Surface-microporous Graphene Sheets, Energy devices

Design and Synthesis of Shape-controlled 3D Carbon Nanomaterials from CO and CO2 with New Alkali Metal Chemistry for Energy Devices

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We developed the novel strategy for the synthesis of shape-controlled 3D carbon nanomaterials based on our discovered reactions between CO/CO2 and alkali metals/oxides [1-5]. With the new alkali metal chemistry, we synthesized various shape-controlled 3D graphene materials from the reaction of CO/CO2. Namely, 3D graphene sheets are generated from CO (or CO2) and alkali metals/oxides with the formation of alkali metal carbonate, which not only served as an isolator to inhibit the restacking of the graphene layers, but also played an in-situ template role in determining the 3D structure of the graphene sheets. Furthermore, a new material□3D surface-microporous graphene was also synthesized from CO2, in which CO2 not only generated 3D graphene sheets from its reaction with alkali metal liquid, but also created the surface-micropores in the produced 3D graphene sheets. In addition, as a hypothetic material with ultrahigh electrical conductivity, alkali-metal embedded carbon nanomaterial was successfully synthesized from the reaction of alkali metal liquid and CO gas. These 3D carbon nanomaterials possess large accessible surface areas and high electrical conductivities, leading to their excellent performance for energy devices (solar cells, fuel cells, batteries, and supercapacitors).

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Abstract ID: 850

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: Water splitting, Nickel phosphide, Topological ferroelectricity, Core-shell

Real-space topological ferroelectricity and self-epitaxial hetero-nanolayers in nickel phosphides

Xiankui Wei[1], Gustav Bihlmayer[2], Yury V. Kolen'ko[3], Lifeng Liu[3], Stefan Blügel[2], Joachim Mayer[1,4], Rafal E. Dunin-Borkowski[1]

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Surface compositional, atomic and electronic structures play key roles in controlling activity of catalysts during electrochemical reactions. As for the supporting matrix, factors such as conductivity, elemental valence state, polyhedral polarity and spin structure [1-3] are also important in influencing performance of the catalysts. However, for earth-abundant and efficient transition-metal phosphides used for water splitting, such atomic-scale structural information is largely missing, which hinders design and optimization of catalysts with superior electrochemical activity. Here, we report the discovery of real-space topological ferroelectricity in non-centrosymmetric Ni2P (space group P-62m). Focusing on polyhedral polarity [4], we establish symmetry equations of polarity and the solution yields that the polarity couples with elemental valence states through nickel atomic sites, which is verified by valence state measurement using electron energy-loss spectroscopy (EELS) and structural characterization. First principles calculations reveal that associated with center-convergent to center-divergent transition of topological geometry under in-plane compressive strain (winding number n = 1), the polyhedral polarity also couples to momentum-dependent spin polarization. The dual roles of nickel cations, i.e., their polar displacements and 3D bonding network, enables the coexisting topological polarity with metallicity [5]. In combination with electron-beam bombardment, our image-simulation-based scanning transmission electron microscopy (S/TEM) study reveals coverage of self-epitaxial Ni2P and NiPx ($0 < x < 0.5$) nanolayers on (001) surfaces of Ni5P4 nanosheets [6]. The discovery of topological ferroelectricity and core-shell scenario in nickel phosphides provide novel insights to understand the catalytic performance of transition-metal catalysts for electrochemical energy conversion.

Key Words: Water splitting, Nickel phosphide, Topological ferroelectricity, Core-shell

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Abstract ID: 851

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Graphene, Mxenes and other two-dimensional materials for energy applications

Keywords: Silicon, Nanosheets, Battery

Ultra-thin silicon nanosheets produced by liquid-phase exfoliation for battery applications

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Liquid-phase exfoliation (LPE) is well adopted by the research community to produce two-dimensional (2D) materials in huge-quantities from layered bulk structures held together by weak Van-der Waals forces [1]. However, our recent work has shown, it can also be applied to specific non-layered materials having unusual mechanical properties or anisotropy to produce nanosheets from non-layered covalent bonded materials [2]. Here, we demonstrate that a combination of pre-treatment and bath sonication of silicon bulk crystals, results in production of ultra-thin silicon nanosheets. The nanosheets produced have length (L) in tens of nanometer with thickness (t) of only a few atomic layers, giving it a high aspect-ratio (L/t) of larger than 20. We want to emphasize here that such high aspect-ratio in nanosheets produced by LPE has only been reported in layered materials so far [3]. Further, silicon is a very promising lithium-ion battery anode material with high theoretical capacity of 3780 mAh/g. Therefore, our work in underway to employ these LPE produced silicon nanosheets as lithium-ion batteries anodes to test the performance. These findings will be of great interest to expand the list of two-dimensional materials that can be produced by this simple cost-effective LPE process.

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Abstract ID: 852

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: Borophene, Electronics, Finite Element, PEDOT:PSS, Polymer Nanocomposite

Effect of Borophene on the elastic modulus and electrical conductivity of PEDOT:PSS. A numerical study.

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The growing need for portable electronics has propelled the collaborative effort from the academia and the industry to develop pseudocapacitive nanocomposites for energy storage applications. However, this endeavor remains quite challenging with use of borophene due to low scale production. Therefore, we employ finite element method to investigate the interaction of 2D boron sheets on the mechanical and electrical properties of Poly(3,4-ethylene dioxythiophene): poly(styrene sulfonate) PEDOT:PSS. This nanocomposite offers enhance electron pathways owing to the synergistic effect of the high transport properties of borophene sheet and the pseudocapacitive behaviour of PEDOT:PSS. Besides, the reinforcing effect of the inclusion in the crosslinked PEDOT:PSS film offers a promising electrode with improve mechanical stability. Consequently, this intriguing result makes borophene/PEDOT:PSS nanocomposite to be highly promising for further investigation and application in cutting edge devices such as touchscreens, thermoelectric, light-emitting diodes, electrochemical, photodiodes, sensors, solar cells, and electrostatic devices.

Abstract ID: 853

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster/Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: chalcopyrite, bismuth, hydrogen, water splitting

Enhancing solar-to-hydrogen efficiency by bismuth-doping in CuGaSe2 photocathodes

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CuGaSe2 (CGS) is a wide bandgap (1.7 eV) chalcogenide p-type semiconductor. It is an attractive candidate for photocathodes in photoelectrocatalytic water splitting because of its high absorption coefficient (α ~ 104 cm-1)[1]. Although bare CGS has been reported as a stable material for water reduction, even in acid conditions, the onset potential is only ~0.130 VRHE due to its too low flat band potential (~0.55 VRHE). It can be associated to the pinning of the Fermi level due to a high concentration of GaCu deep defects[2]. In this work, Ga3+ in CuGaSe2 was partial substituted by Bi3+ expecting to suppress or decrease the concentration of the detrimental deep donors. Bi-doped CuGaSe2 photocathodes were fabricated by a bottom-up all-solution processed approach. The chalcopyrite films were deposited by spin coating from a solution containing 1.25 mol L-1 salts chlorides and 3.5 mol L-1 thiourea in DMF on FTO substrate, with Bi/(Bi+Ga) = 0.5%. The precursor films were selenized at 540 oC during 20 min. Further, 40 nm CdS was deposited by CBD, a ~100 nm TiO2 was deposited by spin coating a solution of Ti(IV) isopropoxide. Finally, Pt was photoelectrodeposited, to act as a co-catalyst. A photocurrent of 11 mA cm-2 at 0 VRHE was registered for water splitting in 0.5 mol L-1 H2SO4 on the photocathode FTO/Cu(Ga,Bi)Se2/CdS/TiO2/Pt under 100 mW cm-2 illumination. This value is tenfold the photocurrent on FTO/CuGaSe2/CdS/TiO2/Pt. Furthermore, the onset potential for the photocathode of Cu(Ga,Bi)Se2 is 0.65 VRHE, which is ~300 mV higher than that obtained with the non-doped CuGaSe2 electrode. The flat band potential was calculated from the curves of Voc versus light intensity. Bismuth-doping caused an increase of ~180 mV in the flat band potential. It suggests that bismuth doping may have suppressed the GaCu deep donors, resulting in a higher onset potential, and, consequently, enhancing the solar-to-hydrogen efficiency (1.92% at 0.3 VRHE).

Key Words: chalcopyrite, bismuth, hydrogen, water splitting

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Abstract ID: 854

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Electrical properties of graphene, Mxenes and other two-dimensional materials

Keywords: Nanoelectronics, Nanostructures, Semimetals, Semiconductor

Semimetals for Nanoelectronics Applications

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The electronics industry has relied for over fifty years on shrinking transistor geometries for improvements in circuit performance while reducing cost per function. The conventional idea of using a fixed material set and scaling devices in length as expressed by Moore's "law" [1] to reduce costs while enhancing the performance came to an end effectively during the mid-1990s for the manufacture of integrated circuits relying on field-effect transistors (FETs). As miniaturization continues to ultra-scaled transistors, the concept of doping to form junctions fails and forming heterojunctions becomes extremely difficult. In semimetals on the other hand, quantum confinement induced bandgap leads to a semimetal-to-semiconductor transition which can be utilized as a novel means for making dopant-free monomaterial rectifying junctions and forming a FET near atomic dimensions. These properties open up new opportunities in bandgap engineering for future nanoelectronic devices.

For atomic-scale device lengths, applying classical continuum models, e.g., the Ohm's law, will no longer be valid and quantum mechanics must be applied to describe the electron transport correctly. This makes nanoscale components conceptually different from larger devices as device dimensions approach the Fermi wavelength of the electrons. Schottky barrier at the interface of bulk-like 'source and drain' regions, and quantum confined 'channel' region in a monomaterial film allows for forming Schottky barrier transistors with critical dimensions of a few nanometer using techniques consistent with advanced nanoelectronics manufacturing.

Our recent studies on semimetal nanostructures, demonstrate that ultra-thin Bi films and semimetallic transition metal dichalcogenides (TMDs) such as PtSe2 and PtTe2 have distinct thickness-dependent electronic structures and physical properties [2-5]. Although the bulk crystal is a semimetal with an overlap of the conduction and valence bands, monolayer PtSe2 and PtTe2 have been revealed to be a semiconductor. The possibility of making semimetal hetero-dimensional junctions with uniform chemical bonding at the interface promises the possibility of fabricating ideal Schottky barriers [6,7].

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Abstract ID: 855

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Graphene, Mxenes and other two-dimensional materials for biomedical and healthcare applications

Keywords: cancer; ball milling; sonication; 2D materials; phototherapy

Photosensitizer and anticancer drug-loaded 2D nanosheets: Preparation, stability and anticancer property

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We have been developing the methods for 2D nanosheet preparation through exfoliation of the bulk materials with an exfoliant by liquid phase sonication and solid phase ball milling. Recently, liquid phase exfoliation was applied to graphite with chlorin e6 (Ce6) as an exfoliant and a photosensitizer to give graphene-Ce6 nanocomposites. The resulting G-Ce6 exhibited significantly improved (7-75 times higher) phototherapeutic efficacy to kill cancer cells in comparison with other previously reported nanomaterial-Ce6 composites. Although G-Ce6 was stable in phosphate-buffered saline (PBS), Ce6 was rapidly released in a cell culture medium, which likely decreases the in vivo efficiency of this composite. In view of in vivo application, we investigated other nanocomposites than G-Ce6 by combining graphene with photosensitizers such as pheophorbide a (Pa) and bacteriopheophorbide a (bPa), and MoS2 nanosheet with Ce6, Pa and bPa. We have also extended the direct preparation methodology of nanocomposites to load anticancer drugs such as doxorubicin and irinotecan in place of the photosensitizers. Herein, we report improved cancer killing efficiency of Ce6 loaded MoS2 (MoS2-Ce6) in comparison to other Ce6 loaded nanosheets including G-Ce6. The high efficacy can be attributed to enhanced photothermal effect of MoS2 as well as photodynamic effect of Ce6 simultaneously.

Abstract ID: 856

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanomaterials and Nanotechnology

Keywords: Biodegradable Electronics, Stretchable Electronics, Metallic Glass

Stretchable Biodegradable Metallic Glass for Transient Electronics

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The recent serious pollution of the soil and ocean by plastic waste provides the lesson that useful and long-lasting inventions sometimes lead to unexpected side effects. The rapid development of electronic devices is now producing excessive electronic waste (e-waste) of toxic or complex materials that are difficult to recycle. In particular, advances in soft and stretchable forms of electronic devices leading the rapid development of biointegrated electronics will bring a severe increase in e-waste. Biodegradable electronic devices are attracting attention as a technology capable of environmentally friendly disposal after their reliable functions are complete. The key idea here -- that even slowly degrading material can be made decomposable in a brief time frame by scaling down material thicknesses at nanoscale -- accelerates the development of biodegradable electronic or transient electronics.

This presentation will spotlight the latest application examples of biodegradable electronics in biomedicine. An amorphous nanoscale metallic glass will be introduced that is both biodegradable and stretchable as an electrode. An electrode of biodegradable metallic glass composed of Ca, Mg and Zn showed elastic strain and fatigue properties superior to those of conventionally structured metals owing to fewer crystalline defects. Integration with other biodegradable layers such as silicon nanomembranes, silicon oxides and PBAT offers various applications in passive and active electronic components as well as a fatigue-resistant triboelectric nanogenerator. Cell toxicity and in-vivo histology results revealed the biocompatibility of this material for use in biointegrated devices.

Abstract ID: 857

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster/Oral Presentation

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: D Nanosheets, Exfoliation, Triphenylene, Dispersion

An efficient and scalable production of 2D material dispersions using hexahydroxytriphenylene as a versatile exfoliant and dispersant

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Since thin layer 2D materials have been attracting enormous interest, various processes have been investigated so far to obtain these materials efficiently. In view of their practical applications, the most desirable source is the pristine bulk material with stacked layers such as pristine graphite. On their exfoliation, we have many options in terms of conditions such as wet or dry, with or without additive, and kind of solvent. In this context, we have found versatile exfoliant, 2,3,6,7,10,11-hexahydroxytriphenylane (Fig. 1), which works efficiently for exfoliation of typical 2D materials, graphene, MoS2, and h-BN, in both wet and dry processes using sonication and ball-milling, respectively, in aqueous and organic solvents.

As for graphene, stable dispersions with relatively high concentration (up to 0.28 mg/mL) in water and tetrahydrofuran were obtained from graphite in presence of hexahydroxytriphenylene by wet process using bath sonication and via dry process using ball-milling. Especially, most of graphite was exfoliated and dispersed as thin layer graphene (Fig. 2) in both aqueous and organic solvents through ball-milling even at large scale (47 - 86% yield). In addition, the exfoliant can be easily removed from the precipitated composite by heat treatment without disturbing the graphene structure. Bulk MoS2 and h-BN were also exfoliated in both wet and dry processes. As in graphene, MoS2 and h-BN dispersions of high concentrations in water and DMF were produced in high yields through ball-milling.

Abstract ID: 858

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster/Oral Presentation

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: 2D Nanosheets, Exfoliation, Ball Milling, Dispersion, Sodium Cholate

Readily Available "Stock Solid" of MoS2 and WS2 Nanosheets through Solid-Phase Exfoliation by Ball Milling

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In this paper, we report simple, scalable and high-yield production of MoS2 and WS2 nanosheets through solid phase exfoliation using ball milling in the presence of sodium cholate (SC). The exfoliated MoS2 and WS2 nanosheets are stored as "stock solid" and readily dispersed in water simply by shaking with hand prior to use. While solid phase exfoliation using ball milling has been applied to the production of graphene nanosheets, this methodology has not been demonstrated in the exfoliation of TMDs such as MoS2 and WS2. Although we have reported scalable method using hexahydroxytriphenylene as an exfoliant through ball milling, bath sonication for half an hour has been required to obtain stable dispersion. As compared with wet-grinding and liquid phase ball milling, the dry process reported here is considered to be more preferable to keep the solid as it is for longer time, because the presence of liquid may facilitate aggregation as mentioned above. In addition, simple dispersion with controlled concentration can be prepared from the dry ball milled solid, while the liquid used for exfoliation under wet conditions may make solvent system complicate, and concentration less precise and less controllable.

First, the effect of surfactant amount in the ball milling process was studied; the amount of MoS2 was fixed at 0.20 g and the amount of SC was varied from 0.010 to 0.40 g. The powder obtained after ball milling was dispersed in deionized water (100 mL) and the resulting dark-greenish suspension was centrifuged at 3000 rpm (1025g) for 60 min. The top 75% of the supernatant (Fig. 1a) was subjected to UV/vis spectroscopic analysis. The yield, the mean number of layers, and lengths of the napnosheets were calculated using the extinction and the reported coefficient at 345 nm, the wavelength of the exciton peak (A), and the ratio of the extinction at 605 and 345 nm (Ext605/Ext345), respectively. As shown in Fig. 1a and 1b, the yield of MoS2 increased according to the increase of the weight ratio of SC/MoS2. The yield of 9% obtained at the SC/MoS2 weight ratio of 2 is much larger than that obtained by liquid phase sonication. The morphology of MoS2 nanosheets was determined to be two layers and 60 - 80 nm in size, from the A observed at 658 nm and the value of Ext605/Ext345.

Abstract ID: 859

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Manufacturing and formation techniques
Keywords: 3D Printing, Grain Boundary Engineering, Fatigue/Creep Interaction, Polycrystalline Material, Inclusion-Void

Modelling Damage in Grain Engineered Voids, Precipitate and Microstructural Distortions during 3D Printing Process

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Additively Manufactured (AM) parts exhibit cracks, low toughness, low plasticity, and high residual stresses. To mitigate these characteristics, a process for grain microstructure in AM alloys is desirable. Integrated Computational Material Engineering (ICME), tools can guide the AM process and predict thermo-mechanical, fracture-fatigue behaviour and altering the process parameters to predict microstructural change. Furthermore, the modelling is needed to predict effect of defects, and inclusions effect on mechanical properties that are important to take AM to mainstream component applications. The microstructures resulting from 3D printing processes of engineering alloys are complex in nature and are effectively the result of micro-welding processes which leave, voids, precipitates, distorted grains, and residual stresses in the process. The 3D techniques are being continuously developed to improve creep/fatigue and oxidation strength of components. Furthermore, these more complex microstructures due to the new fabrication methods mean that a whole new approach is needed in the material testing verification as well predictive modelling to optimize both the laboratory testing and operational processes in components. In this effort grain boundary engineering (GBE) multi-scale modelling of stainless steel is performed to expedite qualification process for existing and new AM polycrystalline alloys. ICME develops a procedure for a meso-scale grain/grain boundary engineered model to simulate the progressive 3D printing process and predict the generation and progressive effects of void and precipitate on the mechanical properties of engineering alloys. Material properties from a representative steel is used to validate the model. In this model micro-cracks can randomly initiate and grow under a micro-triaxial stress state at positions where accumulated damage reaches critical values. Grain size/distortion and void/precipitate density and distribution simulations are shown as a likely reason for crack branching and growth. The model sets out a novel approach and points the way for analysis of more complex microstructures with different phases and sub-grain particles. The development of such models is likely to be the preferred approach to predict 3D manufactured material properties as well as component failures.

Abstract ID: 860

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: Energy Harvesting, Thermoelectricity, Single Molecules, vdW heterostructures; Gold Clusters

Atomic-scale vdW Heterostructures Formed by Gold Clusters and Graphene for Thermoelectric Energy Recovery and Cooling

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Quantum engineering of electrical properties of nanoscale materials is fundamental to the development of high performance thermoelectric devices for the conversion of waste heat into electricity and cooling [1-2]. Here, we demonstrate theoretically that quantum interference [3-4] can be utilized to improve the room temperature thermoelectric efficiency of atomic-scale vdW heterostructures formed by metallic clusters and graphene electrodes. We study systematically the electronic and thermoelectric properties of gold clusters consisting of N = 3, 4, 5, 6 gold atoms (AuN) sandwiched between graphene electrodes. We obtain a high Seebeck coefficient in the range of 100–500μV/K in this heterostructures which is higher than that of the best molecular scale junctions. Our calculations shows that resonance transport at graphene electrodes Fermi energy through atomic scale gold nanoparticles leads to a significant improvement of both electrical conductance and Seebeck coefficient. Our finding shows that gold nanoparticle / graphene heterostructures are promising platform for thermoelectric energy harvesting and cooling.

Abstract ID: 861
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Nanocomposites
Keywords: Environmental DNA, eDNA, sorbent, nanocomposite

A Novel Nanocomposite Sorbent for the Capture and Concentration of Environmental DNA

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Despite the promise of the environmental DNA (eDNA) testing technology in monitoring aquatic life and diseases, and the advancement in eDNA analysis techniques (qPCR, genome sequencing), the wide adoption of eDNA testing is hindered by a lack of an efficient and reliable eDNA sampling tools. Testing laboratories still use regular cellulose or polymer filters for eDNA filtration. Because of their reliance on pore size, these filters face clogging issues, are unable to efficiently capture free, viral, microbial or cellular DNA, thus dramatically lowering the sensitivity and reliability of subsequent DNA analysis. Here, we introduce a new sorbent technology for the collection, concentration and recovery of aquatic viral and microbial eDNA.

The sorbent is a porous nanocomposite material capable of capturing DNA through affinity and specific chemical interactions, thus enabling larger flow rates and efficient capture and recovery of free and microbial eDNA. This enabling technology allows the capture of 10 times mores eDNA and microorganisms, is 10 times faster than traditional methods, and enables large volume analysis without an increase in cost. Such development is expected to enhance ecosystem monitoring, and trigger a rapid growth of the eDNA testing market.

Abstract ID: 862

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Sensors and MEMS: Materials and Devices

Keywords: Thermoelastic damping, energy dissipation, material length scale parameter, dimensionless bending rigidity ratio

Impacts of Size Effects on Material Dependent Dimensionless Bending Rigidity Ratio in Vibrating Rectangular Microplates

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Micro/nano-based rectangular plates are widely used as sensors in the MEMS industry. Among the different energy dissipation mechanisms that exist in resonators, thermoelastic damping is a critical one that limits the maximum achievable quality factor (Q_TED). When the devices were scaled down, it is essential to include size effects also in the analysis. The impact of scaling effect on bending rigidity ratio in micro rectangular plate-based resonators using five different structural materials-Si, polySi, GaAs, diamond, and SiC was analyzed in this paper. The consequences of the scaling effect on Q_TED were found to be remarkable, and Q_TED is significantly enhanced due to changes in bending rigidity ratio. The relation between the size effect parameter (l/h) and the bending rigidity of the microplate was explored and found to be increased. The material order in which bending rigidity varies with dimensionless length parameter was investigated for the five structural materials. The variations in bending ratio with different transitions in l/h were also explored. The analytical study of the energy dissipation reduction technique was realized using various structural materials with different bending rigidity ratios. The simulations were done with MATLAB 2015.

Abstract ID: 863

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Natural Fibre Composites

Keywords: Kenaf, Pineapple leaf, Natural fibre

Investigation of Mechanical Properties of The Hybrid Pineapple Leaf and Kenaf Fibre Composite

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Natural fibres nowadays been famously investigated as alternative fibres due to the source depletion of petroleum. There are several natural fibres such as jute, hemp, sisal, kenaf and pineapple leaf that been actively researched in terms of their mechanical properties. This research was focusing on two of the natural fibres which are the kenaf and pineapple leaf. The kenaf and pineapple leaf fibres were proved by previous researchers to have good mechanical properties. The purpose of this research was to study the mechanical properties of both fibres and also conducting analytical review on chemical composition for kenaf and pineapple leaf fibres. In this study, the single fibre tensile test was conducted using the universal testing machine, using paper frames and adhesives. Besides that, an analytical review from previous researches also been conducted on both fibre's chemical compositions, covering the raw and treated fibres. The single fibre tensile test concluded with the pineapple leaf fibres having higher maximum tensile force than kenaf, and the stress – strain diagram also been constructed. Moreover, as for the analysis review on the chemical compositions of the fibres, it was proved that the treated fibres possess higher mechanical properties than the raw fibres, however the alkaline treatments also need to be controlled so that the properties do not degrade

Abstract ID: 864

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Smart Composites

Keywords: Carbon Fiber Reinforced Polymer (CFRP), Smart Multifunctional Composite, Printed Electronics, Structural Health Monitoring (SHM), Electroluminescence

Smart Carbon Fiber Composite Structures Utilizing Printed Electronics

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Carbon fiber reinforced polymer (CFRP) composites are becoming increasingly common for applications such as aerospace, automotive or construction due to their superior mechanical properties. However, one challenge is predicting the failure of CFRP structures under real-world operating conditions due to the complex structure of woven or braided carbon fibers embedded in a polymer resin. This can be overcome by in-situ monitoring of the strain and damage state of CFRP structures. The carbon fibers themselves can be used for this purpose since they are electrically conductive. However, woven carbon fibers in CFRP act essentially as a uniform 2D conductor, which has limited uses for measurements that require location specificity. In order to create smart CFRP structures, the carbon fibers need to be integrated with other electrically functional materials that are patterned to achieve location specificity or other desired functionality. To do so with traditional electronics manufacturing technology is difficult and expensive. Conversely, printed electronics is well suited to this application as it is inherently compatible with fabricating large-area electronic systems on non-traditional substrates.

In this talk, we will discuss our recent progress creating smart CFRP structures by printed electronics. We will show a process of printing electrodes directly onto woven carbon fibers that are subsequently infused with epoxy resin to create 3D CFRP structures. One application of these contacts is to create self-heating CFRP for aircraft de-icing. We will also show how CFRP damage can be detected using printed contacts whose location has been carefully designed together with the measurement protocol and data read-out circuit to achieve location specificity. More complex multi-layer devices can also be fabricated on CFRP structures. We have fabricated electroluminescent devices where the electrodes are a structural carbon fiber weave and a transparent carbon fiber veil. This can be used to light up CFRP structures as well as visually detect the location of strain and damage. These proof-of-concept demonstrations showcase the power of integrating CFRP with printed electronics to create many other forms of smart CFRP structures in the future.

Abstract ID: 865

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Metamaterials and Materials for THz, Plasmonics and Polaritons

Keywords: Halide perovskites, Nanophotonics, Nanofabrication

Halide perovskites for applications in nanophotonics

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Nanophotonics and meta-optics based on optically resonant all-dielectric structures is a rapidly developing research area driven by its potential applications for low-loss efficient metadevices. Recently, the study of halide perovskites has attracted enormous attention due to their exceptional optical and electrical properties. As a result, this family of materials can provide a prospective platform for modern nanophotonics [1] and meta-optics [2], allowing us to overcome many obstacles associated with the use of conventional semiconductor materials. Here, we overview the recent progress in the field of halide perovskite nanophotonics starting from single-particle light-emitting nanoantennas [3,4] and nanolasers [5] to the large-scale designs working for surface coloration, anti-reflection, and optical information encoding [6-8].

Abstract ID: 866

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: Graphene oxide; CeO2-ZrO2; Nanocomposite; anticorrosion coatings; hydrophobic surface; Interfacial interaction

Fabrication of ceria-zirconia decorated graphene oxide for obtaining a high performance epoxy nanocomposite film with excellent anti-corrosion/mechanical properties

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This research focuses on the synthesis and modification of graphene oxide (GO) nanosheets with ceria-zirconia hybrid nanoparticles. The main aim is to take the advantages of both graphene oxide and ceria-zirconia in enhancing the long-term performance of nanocomposites. For this purpose, the synthesized graphene oxide was treated with ceria-zirconia hybrid nanoparticles. The modified GO hybrid nanosheets were characterized by Fourier transform infrared spectroscopy (FTIR), Field Emission scanning electron microscopy (FE-SEM), X-ray diffraction analysis (XRD), Ultraviolet–visible spectrophotometry (UV–Vis) and Raman spectroscopy. The effects of intercalation of GO sheets, CeO2-ZrO2 and GO/CeO2-ZrO2 nanohybrids on the corrosion protection and barrier performance of the epoxy coating on mild steel were also investigated in natural seawater by electrochemical impedance spectroscopy (EIS) and scanning electrochemical microscopy (SECM). The optimum percentage of ceria-zirconia embedded GO nanoparticles in the epoxy coating (unmodified and triazole modified) was 1.0 wt% in which the coating has minimum agglomeration and appropriate corrosion resistance. The EIS data indicated that the coating resistance of epoxy/CeO2-ZrO2 hybrid nanoparticles-modified GO after 480 h immersion in natural seawater is higher than epoxy/unmodified GO nanosheets. SECM analysis confirmed that the dissolution of Fe2+ was suppressed at the scratch on the coated mid steel due to the higher resistance for anodic dissolution of the substrate. The water contact angle (WCA) results confirmed the reduction of the hydrophobic nature of the surface after the incorporation of GO/ CeO2-ZrO2 hybrids. SEM/EDX analysis showed that Ce and Zr were enriched in corrosion products at a scratched area of the coated steel after corrosion testing. FIB-TEM analysis confirmed the presence of the nanoscale oxide layer of Ce and Zr in the rust of the steel, which had a beneficial effect on the corrosion resistance of coated steel by forming protective corrosion products in the wet/dry cyclic test. The improved mechanical properties were noticed for the nanocomposite coatings containing CeO2-ZrO2 hybrid nanoparticles-modified GO nanosheets.

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Abstract ID: 867

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Sensors and MEMS: Materials and Devices

Keywords: Heteroligand, Plasmon Coupling, Small Target

Detection of small targets using heteroligand-funtionalized plasmonic particles.

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Detecting small target biomolecules, chemicals, or ions is a challenge that requires unique solutions. Most sensing mechanisms especially that of label-free methods rely on minimum level of molecular size, which typically tens of kDa, exerting significant biophysical impact of its presence. Here we describe how the use of heteroligand, instead of the usual monoligand system in plasmonic-based detection can increase the efficiency of plasmon coupling (PC), and hence resulted in a better biosensing signal. PC optimally occurs when two plasmonic particles at the vicinity lower than 4 nm distance. This means target that has a diameter within that range is somewhat advantageous to be detected. However, two typical problems would arise; 1) the capturing agent (ligand or bioreceptor) usually dissipates the dynamic space of the detection, and 2) the target, which is usually chiral in nature, not optimally treated as such during the capturing event. Therefore, using a heteroligand system where different ligand is anchored onto different nanoparticles, both setbacks will be minimized. This work will open new avenues for in-situ small pollutants, and metabolites detection that would benefit both environment and healthcare in the near future.

Abstract ID: 868

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Sensors and MEMS: Materials and Devices

Keywords: Chiral material, dispersion, dielectric loss, solar cell, thick lens

Towards Highly Efficient Solar Cell Design Using a Dispersive Chiral Lens

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In recent work, propagation of polychromatic light through a chiral dispersive spherical boundary has been examined via deriving two sets of ABCD transfer matrices for right- and left-circular (RCP/LCP) modes [1-3]. In this work, the first-order dispersive effects via material dispersion manifested through the dielectric permittivity $\tilde{\varepsilon}$ in a spherical lens are considered. A schematic for a chiral dispersive thick lens illuminated by white light is shown in Fig.1. Incoherent white light (sunlight) is spectrally decomposed into the constituent spectral colors. The dispersed light is then incident upon the chiral lens at location do location. The emergent multicolor waves all propagate in the meridional (YZ) plane. Consequently, based on recent work, individual colors are brought to focus by the lens to unique positions displaced in both Z and Y coordinates [4]. In the present scheme, it is proposed that individual solar cell junctions be placed to intercept each color focal points. The expectation is that in this manner, each cell will absorb a single wavelength, and hence will likely operate more efficiently. Additionally, the multi-cell configuration will undergo less thermal heating caused by polychromatic (including possibly infrared and ultraviolet) absorption.

Abstract ID: 869

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Metamaterials and Materials for THz, Plasmonics and Polaritons

Keywords: Chiral materials, permeability, dielectric loss, polarization, Fresnel lens, imaging

A magnetic chiral dispersive Fresnel lens with controllable foci and dual images

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A chiral magnetic material object is a three-dimensional structure which precludes equivalence with its mirror image by rotation and translation. In this paper, we construct a magnetic chiral dispersive Fresnel lens with controllable foci and dual images, as in Fig.1, with a chiral substrate on which the grooves are etched. We intend to examine the case of a groove-in Fresnel lens with foci dependent upon the lens material parameters such as groove radii, phase refractive indices, permeabilities, permittivities, and groove depth. The use of chirality in a spherical thick lens indicates emergence of virtual and real image regimes, separated axially under dispersion based on wavelength, and also controllable anomalous image formation have been recently examined. A comparable extension is made here to a planar, chiral imaging structure based on the concept of the Fresnel lens. In particular, the case of a Fresnel lens structure with groove-in design incorporating chirality, associated dielectric loss is examined and later extended to a dispersive case with first-order material dispersion. Effects of the lens parameters on dual image formation (corresponding to right circular and left circular polarizations (RCP and LCP)), modified multiple axial images and other issues (such as dielectric losses inherent in chirality) under variable magnetic permeability and chirality coefficient κ will be discussed in this paper.

Abstract ID: 870

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Thin Films and Nanomagnets

Keywords: Key words: thin film, chirality, total internal reflection (TIR), evanescence, Brewster effect

Mode Distribution and Spectral Characteristics of Chiral Thin Film Resonators under p- and s-Polarization

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Investigating the mode distribution and optical properties (such as spectral and resonance characteristics) of chiral thin films is holds out much promise in light of the rapid increase in the potential applications of thin films (including antennas, solar cells, batteries and others). The properties of these devices in the presence of chirality present greater analytical challenges. Metamaterials (which include chiral or handed materials) have been the subject of explosive interest over the past few decades because of their ability to manipulate light in both the near- and far-field zones. Also, they allow electromagnetic fields to be strongly confined within a small region, the so-called hot spot, and they are applied to varied fields ranging from molecular sensing and high-gain antennas to optical filters and smart solar cell grids [1]. Propagation across any interface containing a chiral material involves the development of left- and right-circularly polarized (LCP and RCP) modes in the chiral region. We examine chiral thin films with parallel and perpendicular polarization (p- and s-polarization) in particular to examine the differences in their characteristics as slab-type resonators. Recent work in this regard has focused mainly on the s-polarization, and has primarily demonstrated reduction and non-uniformity in mode densities and free spectral ranges. Since dielectric losses are inherent in chiral materials, their impact upon the thin film resonators are currently under further investigation [2,3]. The work will be extended to the case of p-polarized propagation, and also include behavior under first-order material dispersion to examine the thin film resonators in different frequency bands (in particular the visible and near-infrared). Fig.1 shows the Fresnel transmission coefficients at the achiral/chiral interface (ACC) for p-polarization case. Thickness of thin films is another factor that needs to be considered to achieve the best modal fit for specific applications. It is anticipated that thin films under chirality may improve optical properties such as higher transmitted power over wider spectral bands for real-life applications.

Abstract ID: 871

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanoparticles, Nanowires, and 3D Structures

Keywords: metal-enhanced fluorescence (MEF); surface-enhanced Raman scattering (SERS), antenna, hot spots, direct bilirubin (d-BLR)

Composite 3D nanoplatform surface- enhanced Raman scattering and plasmon-enhanced fluorescence detection of serum bilirubin from jaundice

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The metal-enhanced fluorescence (MEF) and surface-enhanced Raman scattering (SERS) spectra data can be collected synchronously based on a hybrid 3D-nanoplatform, which is composed of a nanostructure-based substrate and a nanowire-containing solution kit to provides rich “antenna” and “hot spots” effects responding for enzyme free and electrodeless detection of direct bilirubin (d-BLR). The emission enhancement spectra and Raman spectra of d-BLR results were found that the linear detection range is from 1 to 10 □M with a relatively high R2 value of 0.99992, which can be used for detecting abnormal d-BLR concentration from 5 to 10 □M. The blood serum of MEF and SERS measurement to d-BLR, which can be synchronously collected in one chip, also show linear response ranges with the detection limit as low as 0.5 μM. The results obtained from our label-free MEF and SERS composite nanoplatform reveals the clinical effectiveness and suitability of the developed in fast-accurate diagnosis of jaundice. Eventually, this hybrid 3D-nanoplatform is worth looking forward to develop as a cheap, robust and portable sensing platform to evaluate the future application.

Abstract ID: 872

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Synthesis and preparation of graphene, Mxenes and other two-dimensional materials

Keywords: Carbon Nanotubes, host guest chemistry, Separation

Diameter-based separation of SWNTs through their mechanical interlocking with nanorectangle

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Although mechanical interlocking of SWNTs has attracted considerable attention [1], it has not been used for separating SWNTs. In this work, a new host molecule named “nanorectangle” connecting two nanocalipers by metal was designed, synthesized, and employed for separating SWNTs. After HiPCO SWNTs were sonicated in 2-propanol followed by centrifugation, the resulting extract showed the red shift in the absorption of nanorectangle (Fig. 1a), indicating its complexation with SWNTs. The mechanical interlocking of nanorectangle was observed in TEM, where two anthracenes attached on the both faces of SWNT (Fig 1b). After removal of host molecule through demetallization, the resulting SWNTs were analyzed by Raman and absorption spectroscopies, revealing the diameter enrichment around 0.9 nm (Fig. 1c). Such high selectivity was also confirmed with (6,5) and (7,6)-CoMoCAT SWNTs. As compared with nanocalipers [2], the better selectivity was observed toward the smaller diameters (Fig. 1c).

Abstract ID: 873

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Multi-scale Modeling of Graphene- and Carbon Nanotube-Reinforced Composites

Keywords: Fatigue life, Carbon nanotubes, Hardness

Fatigue behavior studies of CNTs reinforced Al7075 Metal Matrix composites of brake rotor system

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The multiwalled carbon nanotubes are the superior class of novel materials that has ever discovered in the recent times which imparts excellent mechanical, thermal and electrical properties in the host material when used as the reinforcements. In the present study the nickel coated multiwalled carbon nanotubes reinforced with Al7075 metal matrix composites are subjected to hardness and fatigue studies the reinforcements are added in 0.5%, 1% , 1.5% and 2vol% through squeeze casting technique. The fatigue life was enhanced considerably with the increase in the vol% of carbon nanotubes and for 20% increase in the load carrying capacity with respect to ascast alloy was observed. Sample with 2vol% carbon nanotubes with an ultimate strength of 175MPa gives 1.45E7 cycles fatigue life under the 60% of the ultimate load. The experimental investigation of the fatigue strength is compared using FEA based software and the results are validated. The fractured surfaces are analyzed using SEM images. The Hardness of the composites were evaluated and found that the CNTs reinforcements enhance the HV of the composites.

Abstract ID: 874

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Artificial photosynthesis

Keywords: CO2 reduction, Solar Fuels, Artificial photosynthesis, Energy conversion, photocatalysis

Sustained, photocatalytic CO2 reduction to CH4 by Reduced titania-Cu2O Z-scheme heterostructures

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I would like to introduce recent progress of CO2 reduction research. Photocatalytic conversion of CO2 and water vapor to hydrocarbon fuels is a promising approach for storing solar energy while reducing greenhouse gas emissions. However, still certain issues including low product yields, limited photocatalyst stability and relatively high cost have hampered practical implementation of this technology. In the present work, a unique strategy is adopted to synthesize a stable, and inexpensive photocatalyst comprised of earth-abundant materials: a reduced titania-Cu2O Z-scheme heterostructure. Under illumination for 6 h, the optimized reduced titania-Cu2O photocatalyst enables 0.13 % photoreduction of highly diluted CO2 with water vapors to 462nmol g−1 of CH4 while showing excellent stability over seven testing cycles (42 h). Our studies show the Z-scheme inhibits Cu2O photocorrosion, while its synergistic effects with reduced titania result in sustained CH4 formation in a continuous flow photoreactor. To the best of our knowledge stability exhibited by the reduced titania-Cu2O Z-scheme is the highest for any Cu-based photocatalyst.

Key Words: CO2 Reduction, Solar Fuel, Renewable Energy, Artificial photosynthesis

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Abstract ID: 875

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Bio-inspired design of composites

Keywords: Carbon nanotube, Nano-syringe, Vibration characteristic, Molecular dynamics

A vibration assisted nano-syringe structure using Carbon Nano Tube

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Carbon nanotubes (CNT) having a needle-like geometry with a small radius and good mechanical properties have been attracting much attention as a material for nano syringe in biomedicine and biotechnology area. However, for its practical medical applications, there are a few obstacles that need to be improved: (i) In the process of penetrating the skin (phospholipid bilayer), the needle may cause damage in the skin tissue, (ii) the needle-like geometry of CNT may be clogged by the phospholipid bilayer structure and (iii) the fluidic drug in nano-syringe may get high flow resistance. To overcome these issues, the authors utilized the oscillation characteristics of the multi-wall CNTs. The previous studies reported the multi-wall CNT oscillation characteristics are very sensitive to their initial geometrical or thermodynamical conditions. Therefore, the authors varied initial parameters, such as chirality and external energy source, to get an optimized CNT nano-needle model using molecular dynamics simulations. It is confirmed that the proposed CNT model effectively reduces the puncture force during the lipid bilayer insertion process. In the drug delivery procedure, the effect of vibration on flow resistance is also confirmed. These results presented in this study demonstrate that CNT has great potential in the nano-biomedical industry as a novel syringe material.

Abstract ID: 876

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Epitaxial Materials and Devices

Keywords: Gallium Oxide (Ga2O3), FETs, High-frequency, Harsh-environment

Development of High-Frequency β-Ga2O3 Field-Effect Transistors Aiming for Applications to Harsh-Environment Electronics

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Beta-gallium oxide (β-Ga2O3) has recently gained significant attention as a next-generation power electronics semiconductor owing to its extremely large bandgap energy of 4.5 eV [1] and high breakdown electric field of over 8 MV/cm [2]. The saturation electron velocity (Vsat) in β-Ga2O3 is theoretically predicted to be greater than 1e7 cm/s [3], indicating that β-Ga2O3 field-effect transistors (FETs) are attractive for not only power switching but also high-frequency wireless communications and high-speed logics. In this talk, we will present our development of submicron-gate β-Ga2O3 FETs for applications at high temperatures and/or under strong radiation [4].

We fabricated highly scaled β-Ga2O3 FETs with various gate lengths (Lg) from 50 to 1,000 nm on unintentionally doped Ga2O3 epitaxial layers grown on Fe-doped semi-insulating Ga2O3 (010) substrates by molecular beam epitaxy. The n-type Ga2O3 channel with Si = 4.8e18 cm-3 was formed by Si-ion implantation doping. T-shaped gates were fabricated on an Al2O3 gate dielectric by 100-keV electron-beam lithography and liftoff processes. The source-to-drain distance and the gate width were 2 and 100 μm, respectively.

Superior RF small-signal characteristics of a current-gain cutoff frequency (fT) of 9 GHz and a maximum oscillation frequency (fmax) of 27 GHz were achieved at Lg = 200 nm. Note that the fmax is a record value for Ga2O3 FETs. These high-frequency characteristics are sufficient for applications at frequencies up to 10 GHz, which have been widely used for wireless communications in present-day society.

Delay-time analysis based on the Lg dependence of fT was also performed to investigate an effective electron velocity (Ve) in the Ga2O3 channel region under the gate. The Ve of about 2e6 cm/s was experimentally extracted from a slope of a fitting line on the total delay time versus Lg plot; the value was consistent with the Vsat theoretically predicted.

This work was supported in part by the Strategic Information and Communications R&D Promotion Program (SCOPE) of the Ministry of Internal Affairs and Communications, Japan.

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Abstract ID: 877

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Correlated Electrons

Keywords: Double perovskite, X-ray diffraction, Metal to Insulator transition

Structural studies of NdBa〖Co〗_2 O_(5.75)

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We report here, the temperature dependent structural studies carried out on oxygen-deficient double perovskite NdBaCo_2 O_(5+δ) (δ~0.75). The samples were characterized using x-ray diffraction, dc magnetization techniques. All the diffraction patterns were analyzed using Rietveld profile refinement software. At room temperature (RT) the compound stabilizes in tetragonal structure with space group P4/mmm. Careful diffraction studies reveal the signature of superlattice peaks having the lattice parameters 2apx2apx2cp where ap and cp are lattice parameters of its perovskite structure. The magnetic measurements show transitions at 110 K and 45 K, which corresponds to paramagnetic to ferromagnetic and ferromagnetic to antiferromagnetic transitions, respectively. Reports show metal to insulator transition around 250 K with decrease in temperature. Our detailed structural studies reveal signature of these transitions thereby suggesting significant connectivity between the lattice, spin and electron degrees of freedom that mark the signature of strongly correlated electron system. Understanding this connection will help in unravelling the nature of magnetic behavior and metal to insulator transition and their utility in device applications.

Abstract ID: 878

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: Nanomaterials, electrospinning, polymer composite, breast cancer

Electrospinning of PVA/Chitosin/silver nanoparticles, its characterization, and activity on breast cancer

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In this study, we electrospun the Polyvinyl Alcohol (PVA)/chitosan/silver nanoparticle (AgNPs) solution and observed the effect on breast cancer cell line. As silver is known for its anti-cancer properties and anti-inflammatory effect whereas, PVA/chitosan has good fabrication by electrospinning; the combination has prominence in delivery systems. However, in breast cancer, the proposed activity of fabricated material hasn't been well established. To examine this, the silver nanoparticles were incorporated into the polymer solution. Preparation of AgNPs and their analysis was performed to confirm the size and shape of the NPs formed by dynamic light scattering and transmission electron microscope. Further, UV-visible spectroscopy and Fourier transform spectroscopy substantiated the results. We analyzed the morphologies of PVA/chitosan/AgNPs by scanning electron microscope and AgNPs distribution in fiber mesh by mapping the elements. The high aspect ratio of nanofiber tends to allow controlled release of silver and hence related studies were performed. Biocompatibility and cytotoxicity evaluation of nanofibers was done on the fibroblast cells. We performed the in vitro anticancer activity on the breast cell line to prove our concept. This method can be extended through surface modification and conjugation of silver with various biomolecules, peptides, and pharmaceutical active ingredients.

Abstract ID: 879

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Experimental methods for Composite materials

Keywords: fiber/epoxy, interface, interphase, tensile test, DIC

Interphase characterization of a single glass fiber and epoxy using a tensile test and digital image correlation method

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In this paper, a set-up tensile test for mechanical characterization of glass/epoxy interphase is presented. The test specimens constructed from a single glass fiber embedded in the epoxy resin with the mill scale size. A small testing system is made by the authors in which the tensile test of the specimens can be performed by applying various weights with high accuracy in the range of mg ie.10-5 N and the resulted displacements and strains are measured by digital image correlation (DIC) method in micro or smaller scales.

Using the obtained experimental displacement results for micro tensile tests and by inverse solution of finite element analyses of the specimen, the average interphase mechanical properties can be extracted for glass/epoxy interphase. In this method specimen size is very important and choosing the larger size specimen (similar to standard size) will increase the computational cost or serious difficulties in the problem solving. Therefore, the specimen dimensions should be selected as small as possible.

In the proposed micro tensile test, unlike the nano scale test methods such as nano-indentation, which measure the mechanical properties in a local position, the average interphase properties are calculated along the fiber/epoxy sample interphase, and therefore the obtained mechanical properties are not limited to a specific region of the specimen and preventing the difficulties related to the scattering of results.

The glass/epoxy specimens have a 0.3 × 0.6 mm cross section and a gauge length of 5 mm. A Canon EOS 6D Mark II camera is used for imaging of tensile tests in DIC procedure. On the surface of each specimen a random pattern of spots is created by spraying paint on the sample. After each test, the taken images are used in an image processing software and the distribution map of deformations and strains are evaluated. The displacement results from this step are entered into the FEM analysis and by performing the inverse solution, an average elastic modulus of the interphase region is calculated.

In another attempt and using DIC, strain distribution on the sample surface are obtained and the effect of interphase region on the strain distribution of specimen is also examined. The authors working on these experimental results to present a variable interphase material characterization as well. More details and results will be presented in the full paper.

Abstract ID: 880

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Electrode/electrolyte interface phenomena
Keywords: CO2 reduction, tin-oxide, formic acid

Effects of catalyst morphology of tin oxide-derived on electrochemical CO2 reduction to formic acid

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We investigated the effects of catalyst particle dimensionality on electrochemical CO2 conversion to formic acid in experiments with tin-oxide (SnOx) derived 3D nanoparticles and 2D nanosheets deposited on carbon gas diffusion electrodes. We chose SnOx as the model materials to study because: (1) SnOx are low-cost catalysts, and (2) these catalysts have been extensively studied for CO2R to formate on planar electrodes in H-type electrochemical cells.1, 2 The SnOx nanosheets were synthesized via a hydrothermal method based on the report from Wan et al.3. The electrochemical CO2 reduction was performed in a continuous flow cell electrolyser with the SnOx coated gas diffusion electrode, a Nafion® 117 membrane separator, and commercial IrO2 coated anode. The catholyte and anolyte were both 0.5 M KHCO3.

Our results suggest that a “tip” effect likely exists during the electrocatalysis processes as a result of the limited interfaces between the catalyst materials and conducting carbon substrate. Such effect makes nanoparticles with less contacting area with carbon substrate easier to be reduced and less selective for formate production at current density above 100 mA cm-2 as compared to the nanosheets with extended interface. Consequently, the SnOx nanosheet coated electrode achieved a partial current density 116 mA cm-2 for formate at a cathode potential of -1.03 V versus reversible hydrogen electrode. This paper provides more details and discussion to supplement our prior article.4

Key Words: CO2 reduction, tin-oxide, formic acid

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Abstract ID: 881

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Electrical, optical, electrochemical, thermal and mechanical properties of graphene, Mxenes and other two-dimensional materials

Keywords: Diradical Character, Conjugated Molecules, Nanostructures, Aromaticity

Conjugated Pi-Structures with Different Topologies

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Carbon-based nanostructures have shown revolutionary influence in the areas of chemistry, physics and materials science. Recent efforts have been focused on novel topological structures of sp2-carbons such as carbon nanohoops, nanobelts, molecular cages, and open-shell nanographenes, which provoked new chemistry and materials. However, synthesis of this kind of molecules is extremely challenging mainly due to strain or intrinsic high reactivity. Another issue is that most of these carbon nanostructures have a localized aromatic character; that means, the π-electrons are not globally delocalized along the backbone, which limits their optical and electronic properties and applications. Herein, synthesis of a series of novel pi-structures with different topologies will be introduced, and their physical properties, aromaticity and diradical character will be discussed.[1-11] They include: 1) azulene-embedded linear compounds and curved nanographenes; 2) cyclopenta ring fused bisanthene and its charged species with open-shell singlet diradical character and global aromaticity/anti-aromaticity; 3) zigzag-edged nanographene and nanobelts.

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Abstract ID: 882

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster/Oral Presentation

Topics: Solar Cells

Keywords: Key words: Excited state dynamics, hot-carrier relaxation.

Study of Hot-Carrier Relaxation Dynamics of Cs4CuSb2Cl12.

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In the recent years, metal halide perovskites have emerged as one of the fastest growing photovoltaics technologies. This has achieved lab-scale device efficiency of more than 23% by improving the quality of interfaces, carrier transport layers and perovskite films. Despite this tremendous progress, the organic-inorganic lead halide perovskite solar cells suffer from long-term stability, degradation and toxicity. The perovskite film is very sensitive to ambient humidity, easy to get dissolved and degraded by moisture, and has toxicity issues due to the presence of lead. Although attempts were made to stabilize the lead-based perovskite active layer1 there is an impetus to develop non-toxic alternatives to lead halide perovskites, with improved stability and efficiency for solar cell applications. One of the ways to get the lead-free perovskites is by substituting four Pb2+ cations with a divalent and two trivalent cations, for example, Cs4CuSb2Cl12 (CCSC). This gives rise to double perovskites, which have recently emerged as viable alternatives to lead halide perovskites. Theoretical and experimental studies have demonstrated that CCSC exhibits high photo- and thermal-stability, is tolerant to humidity and its band gap values lie in the range of 1.0-1.79 eV. These properties make CCSC a suitable absorber material in solar cells. Apart from chemical and thermal stability, its magnetic response has also been explored, which shows long range magnetic ordering with anti-ferromagnetic behavior. However, the band-gap nature and excited state dynamics of these microcrystals are yet to be explored.

Here, we have theoretically investigated the electronic band structure, total density of states, dielectric constants and synthesized the microcrystals of CCSC. We have studied the different vibrational modes with Raman activity of this material. Using ultrafast transient absorption spectroscopy, we have explored the relaxation rates and pathways of hot-carriers. An analysis of the hot carrier relaxation process in CCSC will give us valuable information on its intrinsic carrier dynamics and further applications in solar cells.

Key words: Excited state dynamics, hot-carrier relaxation.

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Abstract ID: 883
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Nanocomposites
Keywords: Zinc Sulfide, Theranostics, Sialic acid, STAT3, NIR

Rare earth metal doped nanocomposites for targeted delivery and imaging of cancer cells

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Chitosan (CS), a natural glucosamine polymer reduces the toxicity and improves cellular internalization of chemotherapeutic agents. In the present study we reported the beneficial effects of paclitaxel entrapped CS modified, luminescent rare earth metal based nanoparticles (LNPs) LaAlO3:Bi3+, Tb3+ nanophosphors (CS-PTX-LNPs) for theranostics applications in cancer cells. LaAlO3:Bi3+,Tb3+ nanophosphors were synthesized by polyol mediated technique and characterized by X-ray diffraction, Field emission Scanning electron microscopy (FESEM), Energy Dispersive X-ray Analysis (EDAX) and emission/excitation spectroscopy. Bismuth activated Lanthanum aluminate with codoped terbium nanoparticles were then surface modified with CS to improve biocompatibility and facilitate entrapment of PTX. The cytotoxicity, cell uptake and NIR imaging was assessed in MDA-MB231 breast cancer cells. The results of the present study demonstrated CS-PTX-LNPs have greater cellular internalization and anticancer propensity compared to naïve PTX and blank LNPs. Further these nanoparticles are hemocompatible without having off-target effects. CS-PTX-LNPs, therefore, is a promising multimodal system for therapy and bioimaging (theranostics) of breast cancer.

Keywords: Chitosan, nanophosphors, theranostics, breast cancer, cellular internalization, drug delivery

Abstract ID: 884

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanomaterials and Nanotechnology

Keywords: Zinc Sulfide, cancer, PBA, apoptosis, NIR

Transition metal doped ZnS nanophosphors for targeted cancer theranostics

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Zinc sulphide (ZnS) is a cytocompatible metal, which possess significant luminesce propensity for bio-imaging and drug delivery applications. In our previous study we have found the enhanced photoluminescence of ZnS nanoparticles (ZnS NPs) when doped with transition metal copper (Cu). IR780 iodide is a near-infrared (NIR) dye with a huge potential for cancer imaging and phototherapy (photodynamic therapy/photothermal therapy). However, low cell uptake and off-target effects are the limitations of IR 780 for effective phototherapy in cancer. In addition IR 780 mediated phototherapy activates STAT3 signaling pathway, which again results in survival of cancer cells. In the present study we, therefore, propose transition metal (TM) doped ZnS NPs for targeted combinatorial delivery of IR-780 and STAT3 inhibitor (Stattic) to cancer cells. Phenylboronic acid (PBA) is a ligand, which selectively binds to the sialic acid (SA) receptors overexpress on the surface of cancer cells. We, therefore, hypothesise surface modification of IR 780 and Stattic loaded ZnS NPs (STAT3-ZnS NPs) with PBA (PBA-STAT3-ZnS NPs) will result in selective eradication of cancer cells. The developed PBA-STAT3-ZnS NPs (100 nm) have superior anticancer and bioimaging propensities for prospective applications in cancer theranostics

Abstract ID: 885

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: Few Layer Graphene, Energy Storage, Nitrogen Doping

Synthesis and Characterisation of Few Layer Pristine and Nitrogen Doped CVD Graphene for Supercapacitor Application

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Graphene has been explored extensively due to its astonishing electrical, optical, mechanical and thermal properties. Recently, it gained significant attention in the area of energy storage devices due to its high surface area, low cost and minimal environmental impact. In the current study, we have synthesized few layers pristine and nitrogen doped graphene on copper foils through Low Pressure Chemical Vapor Deposition (LPCVD) assisted approach for supercapacitor application. The FLG samples were transferred through PMMA (Poly(methyl methacrylate)) assisted copper etching method on the desired substrates for further characterisations. The nitrogen presence was confirmed through the SEM-EDS mapping and XPS data revealed the formation of graphitic-N, pyrrolic-N and pyridinic-N bonds.

The supercapacitor device was fabricated by sandwiching the PVA (Poly Vinyl Alcohol) hydrogel Na2SO4 electrolyte membrane between the two FLG samples on copper substrates as electrodes. The cyclic voltammetry and charge discharge characterisations were performed for the estimation of specific capacitance and energy density and power density of the device. Cyclic voltammetry of the symmetric supercapacitor device fabricated by N doped CVD graphene exhibit high areal capacitance in the range of 0.9mF/cm2 to 0.1mF/cm2 at the scan rates ranging from 10 to 500 mV/s respectively.

Nitrogen doping in graphene resulted in the higher areal capacitance due to the enhancement in electrochemical activity in comparison to pristine graphene.

Abstract ID: 886

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Polymeric composites

Keywords: Polyurethane, Hyper-viscoelastic model, Moony-Rivlin, Dynamic loading

Experimental and numerical damage evolution of polyurethane material using a modified hyper-viscoelastic constitutive model

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Recent investigations about the elastomeric polymer composites emphasized the positive effects of the contribution of elastomers to improve the performance of the protective structures. The unique mechanical and thermal properties and also the self-healing capability of this kind of materials make them remarkable to manufacture highly resilient protective systems. Investigations have shown that the performance of the composite structures with elastomeric polymer coating will significantly enhance their deformation and energy absorption capacity. The nonlinear behavior of elastomers makes major challenge in modeling and investigating the performance of these materials under dynamic loading. This nonlinear behavior caused by the long-chain molecular structure leads to hyper-viscoelastic properties of the elastomers. The characteristics of elastomers depend on different factors such as pressure, temperature and applied loading rate. Therefore, the mechanical behavior of elastomers alters by varying the applied loading rate. One of the most useful elastomers in industrial applications is Polyurethane (PU). PU is a hyper elastic and viscoelastic material formed by isocyanates with chemical reacting of polyol. In this paper several PU specimens made of 3 different shore hardness sheets are subjected to the uniaxial tensile loading to modify the Moony-Rivlin strain energy density function with a viscoelastic model. The uniaxial tensile tests are also performed for 3 different shore hardness under varying strain rates regimes (between 0.001 to 0.1). Then the numerical model based on the modified hyper-viscoelastic strain density function is developed. For this purpose a user material subroutine is added to the ABAQUS finite element software. Then the analyses are performed to predict the damage evolution and tearing in the PU specimens. The effects of loading rate and shore hardness are also investigated on damage evolution of the polyurethane material under dynamic loading.

Abstract ID: 887

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Financial and economic analysis of composite materials

Keywords: Additive Manufacturing, Liner, Polyethylene, Cost estimation

Cost estimation of polymer material fabricated by FDM process in biomedical implant

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Human knee implants are having an enormous market due to the increase in the osteoarthritis problem worldwide. This implant is mostly made up of traditional manufacturing processes such as casting, molding, and machining. After the casting process, the product is machined with the assistance of Computer Numerical Control (CNC) turning, milling, and polishing machines to develop the final shape and tolerance limit. In the future, additive manufacturing processes might change the casting of metal and machining used in the traditional manufacture of implants due to the customized design, reverse engineering concept, reduced scrap, and easily manufacture difficult and complex shapes. When calculating the cost of the product developed by the additive manufacturing process, it is not fully framed to commercialize the implants in the market. Therefore, in the current paper, a comparative study is carried out to estimate the cost of the product manufactured by both conventional and additive manufacturing processes. The total cost of the prototype is calculated based on the building cost, which includes material cost, processing cost, machine running cost, labor cost, and post-processing cost. The present research focuses on the cost estimation of liner in the knee implant for the biomedical application, which is predominantly made up of polymer material like polyethylene.

Abstract ID: 888

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Photonic devices and applications

Keywords: Nanostructure, High power, Laser, Threshold current, Response frequency

Investigation of nanostructured high power AlxGa1-xAs/GaAs vertical-cavity surface-emitting lasers

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The objective of this study has been to investigate and to characterize high power 850 nm vertical-cavity surface-emitting laser (VCSEL) using oxidation confinement technique. The active layer was consisted of three pairs of Al0.3Ga0.7As/GaAs nanostructures and it exhibited a photoluminance emission wavelength of 835 nm. Distributed Bragg reflector mirror nanostructures of 40 pairs in n-type and 21 pairs in p-type were designed to confine the resonance. The multi-layered epitaxial wafers were processed by photolithography using photo masks. Inductively coupled plasma etching was employed to create the platform during the mesa process. Various non-oxidized aperture sizes have been achieved by a wet-oxidation method. The experimental results showed that the VCSEL device exhibited low threshold current of 0.6-0.8 mA. The optical output power was about 6.0-6.8 mW at the injection current of 6 mA. The slope of efficiency was found to be about 3.2~3.7 mW/mA. The corresponding voltage was in the range of 1.7~2.1 V. On the other hand, an eye diagram could be clearly observed under the high data rate of 25 Gbit/sec. The response frequency was measured at 17.1 GHz at -3 dB, also at the injection current of 6 mA. In addition, the related electro-optical characteristics have been summarized and would be further discussed.

Abstract ID: 889

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Photonic devices and applications

Keywords: I am highly interested in this conference to upgrade my research skills in this field.

New Functional Pyrene-Pyridine Integrated Hole Transport Materials for Solution-Processed OLED with Reduced Efficiency Roll-off

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New Functional Pyrene-Pyridine Integrated Hole Transport Materials for Solution-Processed OLED with Reduced Efficiency Roll-off

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A series of new functional-pyridine appended pyrene derivatives viz, 2,6-diphenyl-4-(pyren-1-yl)pyridine (Py-03), 2,6-bis(4-methoxyphenyl)-4-(pyren-1-yl)pyridine (Py-MeO), 4-(pyren-1-yl)-2,6-di-p-tolylpyridine (Py-Me), and 2,6-bis(4-bromophenyl)-4-(pyren-1-yl)pyridine (Py-Br) were designed, developed, and studied as the hole transport materials (HTMs) for organic light-emitting diode (OLED) application. The crystal structures of two molecules revealed to have a large dihedral angle between the pyrene and pyridine units indicating very poor π-electronic communication between them due to ineffective orbital overlap across the pyrene-pyridine systems as the two p-orbitals of pivotal atoms are twisted at 66.80◦ and 68.75◦ angles to each other in Py-03 and Py-Me, respectively. The influence of variedly functionalized pyridine units on the electro-optical properties and device performance of the present integrated system for OLED application was investigated. All the materials have suitable HOMO values (5.6 eV) for hole injection by closely matching the HOMOs of indium tin oxide (ITO) and the light-emitting layer. All the synthesized molecules have suitable triplet energies, glass transition, and melting temperatures which are highly desirable for good HTMs. The pyrene-pyridine based devices

demonstrated stable performance with low-efficiency roll-off. The device with Py-Br as HTM showed a maximum luminance of 17300 cd m-2 with a maximum current efficiency of 22.4 cd A-1 and EQE of 9 % at 3500 cd m2 with 7% roll-off from 1000 to10000 cd m-2. Also, the devices with Py-Me and Py-03 showed performance roll-up while moving from 1000 to 10000 cd m-2.

Key Words: Synthesis, Hole- transport materials, OLED,

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Abstract ID: 890

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Correlated Electrons

Keywords: Quantum phase transition, Bad metal behavior

Anomalous high temperature resistivity behavior in Sr1-xCaxRuO3 (x=0,0.5)

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A smeared quantum phase transition can be achieved by doping calcium ions at the A site of the perovskite transition metal oxide SrRuO3. As reported in the literature1, the quantum critical point is best estimated to be around 38% of calcium doping. As revealed by the x-ray diffraction technique, the compounds under study are single phase and stabilize in the orthorhombic, Pnma space group. The dc susceptibility measurements reveal Tc of 164 K and 23 K, for x=0 and 0.5, respectively. These values are in line with the literature. Both the compounds exhibit bad metallic behavior above 300 K. Conventionally, with an increase in Ca doping, the resistivity is expected to increase3 due to an increase in RuO6 octahedral distortion. But in our case, we observe opposite behavior despite the samples being single phase. In addition, we also observe different thermal behavior of resistivity for both compounds. It is important to note that, in the case of resistivity values for the end compounds, there are also contradicting reports3,4. We believe that these behaviors will be helpful in understanding the bad metallic behavior of ruthenates and its effects due to sample preparation conditions.

Abstract ID: 891

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Photonic devices and applications

Keywords: Nanoparticle core-shell structure, Z-Scan, Optical Limiting

Enhanced optical nonlinearity and optical limiting property of ZnS@graphite core-shell structure

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Enhanced optical nonlinearity and optical limiting property of ZnS@graphite core-shell structure

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The protection of optically sensitive devices from laser-induced damage calls for the requirement of nonlinear optical materials with improved optical limiting behavior. Such materials should always maintain the output fluence below the damage threshold even at high input fluences.[1] In this work, we report the enhancement in the nonlinear absorption of ZnS nanoparticles upon the formation of a core-shell structure with graphite. The ZnS/graphite core-shell structure was synthesized in chlorobenzene by the method of Pulsed Laser Ablation in Liquid (PLAL). The UV-Vis spectroscopic studies revealed the absence of the characteristic SPR peak at 270 nm of ZnS nanoparticles confirming the core-shell formation.[2] The nonlinear absorption studies were conducted using the single-beam Z-scan technique and the sample showed Reverse Saturable Absorption (NLA) behavior. The effective NLA coefficient was found to be 35.8×10-10 m/W at 0.138 GW/cm2 which is three-fold larger than that of pristine ZnS nanoparticles.[3] The synthesized ZnS/graphite core-shell structure exhibited an Optical Limiting (OL) threshold value of 0.37 J/cm2 which qualifies our structure for its potential use in optical limiting applications.

Key Words: Nanoparticle core-shell structure, Z-Scan, Optical Limiting

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Abstract ID: 892

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanoparticles, Nanowires, and 3D Structures

Keywords: PET-RAFT, Nano, Self-assembly, Energy, Photochemistry, Upconversion

Synthesis of amphiphilic nanoparticles prepared by PET-RAFT PISA polymerization as confined systems for upconversion

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Sensitized triplet-triplet annihilation-based upconversion (sTTA-UC) is a promising technology for the development of efficient photosensitive devices including photovoltaic, photochromic displays and biological imaging [1]. It is based on a sequence of photophysical processes between two dyes, a sensitizer and an emitter, high quantum yields can be achieved in low viscosity solution whereas the efficiency falls in solid materials. This aspect limits the integration of sTTA-UC systems in devices and their practical use [2]. Our project has the purpose of developing nanostructured polymeric systems where the sensitizer and emitter are confined in a low viscosity core, exploiting photoinduced electron/energy transfer (PET)-RAFT PISA polymerization. This robust and versatile protocol allows the polymerization of complex architectures, such as amphiphilic block copolymer nanoparticles (NPs) in green conditions (room temperature, presence of oxygen and low-toxicity solvents). Metalloporphyrins have been exploited as photoredox catalysts (PCs) for the PET-RAFT synthesis of both solvophilic and solvophobic blocks. Stimuli-responsive and cross-linkable high glass transition temperature (Tg) polymers have been selected for the solvophilic shell; whereas for the core low Tg materials, such as acrylates, are needed. Self-assembly is achieved through polymerization-induced self-assembly (PISA) which results in high solid content (25-50% w/w), making this method suitable to scale-up. The PC migrates into the solvophobic core during PISA and it is encapsulated into the new-formed nanocarrier. In so doing porphyrin acts both as catalyst for the polymerization and sensitizer for the desired application. Finally, the emitter is added to the solution during the self-assembly. The resulted core-shell nanoparticles with a highly mobile core should increase the TTA-UC efficiency in solid state since collision of the two encapsulated moieties will be more likely in nanometer scale volume: each nanoparticle behaves as an isolated up-converting unit. The final nanoparticles can be used in both photovoltaic and biological imaging simply by adjusting the nature of the monomer used, while maintaining the same protocol.

Abstract ID: 893

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: nanocrystalline, perovskite, synthesis, exchange bias

Synthesis, structural and magnetic properties of Eu3+-doped LaFeO3 and Eu3+/Cr3+ co-doped LaFeO3 nanoparticles by mechanosynthesis

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A novel method for the preparation of nanocrystalline particles of single-phased LaFeO3 perovskite-related is realized by mechanosynthesis method. Prolonged milling of initial oxide reactants (La2O3, α-Fe2O3) with subsequent heat treatments. The formation temperature of the resulting perovskite is 400 oC lower than those at which the material is conventionally synthesized. Co-doping with 30% of Eu3+ ions and 5% of Cr3+ ions caused a decrease in the average crystallite size. The Mössbauer measurements revealed that Fe3+ ions are present in all synthesized samples and ordered antiferromagnetically. The spectrum of La0.7Eu0.3FeO3 and La0.7Eu0.3Fe0.95Cr0.05O3 consists of two sextets. LaFeO3 exhibited exchange bias effect with blocking temperature more than 300 K. We find that the lack of magnetic saturation at high temperature is accompanied by irreversibility up to 90 kOe (i.e., hysteresis loops are open). The magnetization was found to increase drastically in the case of La0.7Eu0.3FeO3, while the magnetization of La0.7Eu0.3Fe0.95Cr0.05O3 decreased slightly.

Keywords: nanocrystalline, perovskite, synthesis, exchange bias

Abstract ID: 894

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Photonic devices and applications

Keywords: Zinc sulfide, photodielectric effect, electroluminescence, electric modulus

Photodielectric Polarization of Zinc Sulfide Electroluminescent Layers

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Investigations in the electroluminescence of polycrystalline semiconductors for an alternating electric field are mainly based on the study of AIIBVI compounds. The advantage of these materials is the possibility of direct conversion of electrical energy into light. In connection with this, the study of the electrophysical properties of electroluminophors under various factors of influence is important both for studying the processes occurring and for practical application of electroluminescent structures. The frequency dependences of dielectric parameters of ZnS electroluminescent polycrystalline structures doped with copper are studied in the dark and under light excitation in the visible wavelength range. When studying the influence of illumination on the frequency dependence of the capacitance of the investigated structures on the basis of ZnS : Cu, a photodielectric effect was observed [1, 2], which consists in increasing the capacitance under the action of light excitation. Contribution to the observed photocapacity can also give a change in the charge state of the local energy trapping centers in the forbidden band. This, in turn, leads to the formation of an additional space charge, which increases the capacitance, dielectric losses, and conductivity of the capacitor structures under investigation. So the established nature of the frequency dispersion of the dielectric coefficients can be explained by polarization of the space charge, which is the electrical inhomogeneity that arises in the material and leads to dielectric losses. The frequency dispersion of the dielectric parameters can also be related to polarization of the space charge formed with the participation of copper impurity centers and defects of the polycrystalline structure. The analysis of data indicates they can be correlated with luminance characteristics of an electroluminescent layer. The dielectric relaxation was studied at a constant temperature using the complex electric modulus formalism. It can be assumed that the nature of the dependence of the components of the electric modulus on the illumination of the sample is related to different contributions to the dielectric polarization from both polycrystalline structure grains and their boundaries. The dielectric data clearly indicate the presence of non-Debye type dielectric relaxation in ZnS : Cu with a distribution of relaxation times. The analysis of the influence that illumination has on the frequency dependence of electric modulus components indicates that the observed relaxation process is a photo-induced one.

Key Words: Zinc sulfide, photodielectric effect, electroluminescence, electric modulus

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Abstract ID: 895
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Polymeric composites
Keywords: Recycling, reuse, plastics, environmental pollution

Environmental Protection Through Recyclable, Reusable and Renewable Composite Materials

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The growing awareness of the factors affecting the environment is a welcome development globally. These factors, constantly influence the choice of materials and how materials in general, are used and disposed of. Human lifestyles and the indiscriminate disposal of wastes have contributed largely to the increasingly hazardous environment, leading to various health challenges and constant natural disasters. In the last two decades, several approaches have been adopted in trying to address and ameliorate these complex problems. One of the major contributors to the huge waste generation is plastic-based materials. Plastics remain a major societal benefit to mankind, in innumerable ways, even though there are high environmental and health risks associated with plastics. Plastics are a major pollutant on land and in water bodies. The immense benefits of plastic materials, particularly in the food and packaging industries, medical and health sector, automobile, aviation and the construction industries, have encouraged their continuous usage. This is due to the versatility, low-cost, less production energy when compared to the alternative materials (metal or glass), vis-à-vis, their ease of processability, since they can easily be formed into any shapes and sizes and the tendency to attain different properties, based on manufacturing methods. Due to these qualities and the undeniable importance of polymeric materials, there is a need to develop and improve the recycling and the reuse of plastic materials. This study demonstrates ways of protecting the environment, through recycling and reuse of polymeric-based products, therefore, creating significant benefits to the environment. Highlights are also made with regards to other environmentally-friendly ways and manners of disposing of polymeric-based products.

Abstract ID: 896

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Sandwich materials/hybrids, Multifunctional composite, Advanced composites

Keywords: rotary swaging; clad composite; grain refinement; microstructure

Al/Cu laminated wire conductors; effect of stacking sequence on mechanical properties and structural features

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Research and development in virtually all the industrial fields has led to the emergence of numerous modern components, as well as to the introduction of a variety of innovative materials, among which are also modern clad composites [1]. The presented study deals with the preparation of Al-Cu clad composite wires with two different stacking sequences via the intensive plastic deformation technology of rotary swaging (RS). The aim of the work was to provide characterization of the effects of RS on selected structural features and mechanical properties of the composites and their metallic components. The results showed that fine more of less equiaxed grains with no prevailing preferential orientations were present within all the Al and Cu composites' components of the final 5 mm thick wires, which points to the occurrence of dynamic recovery/recrystallization during processing. Grains misorientations were locally present primarily in the Cu components; the Al components did not exhibit any substantial presence of misorientations, which is in accordance with the observed structure relaxation. The tensile tests of the swaged composites revealed both the stacking sequences to exhibit comparable ultimate tensile strength of almost 280 MPa. However, the ductility differed notably; the very low ductility of the composite consisting of Al sheath and Cu wires corresponded to the significant work hardening of the Al sheath, as also documented by the relatively high average microhardness of the Al sheath.

Abstract ID: 897

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: IrRu Electrocatalysts, Oxygen Evolution, PEM Water Electrolysis

Efficient and durable oxygen evolution reaction for proton-exchange membrane water electrolysis enabled by iridium-based nanocluster catalysts

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Proton exchange membrane water electrolysis (PEM-WE), compared to conventional alkaline water electrolysis (AWE), shows many advantages such as more compact configuration, higher energy efficiency, larger maximum current densities, higher H2 purity, and dynamic flexibility of operation [1]. However, the rapid degradation of catalysts in the strongly acidic and highly oxidative environment severely limit the materials of choice. By far, iridium (Ir) based materials are the best performing electrocatalysts capable of catalyzing the oxygen evolution reaction (OER) in the acidic solution [2]. To enable widespread deployment of PEM-WE technology, the OER performance of Ir-based catalysts must be drastically improved and meanwhile the Ir utilization should be kept as minimal as possible.

In this presentation, our recent effort toward developing efficient and durable IrRu alloy nanoclusters will be presented. We developed a one-pot hydrothermal approach to the synthesis of ultrafine IrRu alloy nanoclusters loaded on conductive, acid-stable, amorphous tellurium nanoparticle support (IrRu@Te, Figure 1) [3], and the as-obtained IrRu@Te catalysts show a mass activity of 590 A gIrRu-1 at an overpotential of 270 mV and good catalytic stability in strongly acidic electrolyte (i.e., 0.5 M H2SO4) with respect to other control catalysts, due to the large exposed electrocatalytically active surface of ultrafine IrRu alloy nanoclusters and the strong electronic coupling between IrRu and the support. In addition, we managed to grow IrRu alloy nanoclusters homogeneously on metal organic framework (MOF) derived carbon support (CoCN) [4], which exhibit even higher mass activity (2041 A gIrRu-1 at an overpotential of 300 mV) and better catalytic stability in 0.5 M H2SO4. Both catalysts are also active in neutral solution and show improved stability.

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Abstract ID: 898

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanomaterials and Nanotechnology

Keywords: magnetic nanoparticles, NMR relaxivity, nanomagnetism

A fistful of chemico-physical parameters crucial for 1H-NMR relaxation: the effect of size, shape and coating in iron oxides core-shell nanoparticles

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An increasing awareness about novel medical applications of smaller, inorganic-based nanoparticles, possessing unique properties at the nanoscale, has led to a burst of research activities in the development of “nanoprobes” for diagnostic medicine and agents for novel, externally activated, therapies. In this research field, magnetic nanoparticles (MNPs) are prominent due to fundamental peculiar properties which make them particularly appealing to materials and biomedical applications.

In particular, much attention was devoted to MNPs useful as agents for Magnetic Resonance Imaging (MRI), Optical Imaging (OI) and Magnetic Fluid Hyperthermia (MFH), carriers for drugs and vectors for molecular targeting. The possibility to collect images of the regions where the MNPs are delivered through MRI and eventually OI (if functionalized with a luminescent molecule), is joint to their use under radio-frequency fields, with frequency of the order of 100 KHz, which causes a local release of heat directed to tumour cells (the MFH effect), possibly inducing their death. By such materials, theranostic agents can be obtained. On the other hand, in the field of drug delivery and molecular targeting, few examples of reproducible experiments using superparamagnetic nanoparticles are actually present in literature. Thus, the applications of MNPs to nanomedicine is currently of growing interest in the world.

The main objectives of my research group in the last decade was to contribute to the knowledge of physical mechanisms at the basis of MNPs used in biomedicine (especially MRI) and to propose some novel systems in strict collaboration with different research groups of chemists and biologists. I will present a mini-review of different case studies [1-4] where I show how the chemico-physical characteristics of MNPs are strictly correlated to their properties and can be partially interpreted with the most famous heuristic model [5] used in literature for NMR relaxivity profiles.

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Abstract ID: 899

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster/Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: fluorinated, tin oxide, oxygen defects, charge transport, photoelectrochemical cell

"Less-defective" Fluorinated SnO2 as Charge Transport Layer in Photoelectrochemical Cells

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Optimum charge transport within layers is one of the critical features for the efficient performance of various optoelectronic devices. In this work, fluorine doped tin oxide (F-SnO2) film is synthesized by a straightforward and handy solution-processable method using SelectfluorTM (F-TEDA) for efficient charge transport layer. The mechanism of fluorine doping (~2.5 atomic%) and its effects on oxygen defects and electronic band- structure are thoroughly analysed using X-ray and ultraviolet photoelectron spectroscopy. Substitutional doping is observed throughout the depth; however, interstitial doping decreases and finally extinguishes along the depth of F-SnO2 films. F-SnO2 films exhibit more than one order higher conductivity, decreased oxygen defects (~80%), and an increased donor density (65%), making it suitable for a charge transport layer in photoelectrochemical cells (PEC). F-SnO2 as a charge transport layer in a typical PEC cell in aqueous neutral medium showed an ~81 % increase in the photocurrent density (at 1.6 V versus RHE), and electrochemical impedance spectroscopy (EIS) analysis showed a ~36% decrease in charge transfer resistance in comparison to pristine SnO2 films. Thus, the efficient transport of photogenerated charges is observed with minimal recombination losses for “less-defective” fluorinated SnO2 films. This work opens up the door for defect passivation via single-step fluorination of metal-oxide based charge transport layers for optimum utilization in a plethora of optoelectronic devices.

Abstract ID: 900

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Magnetization Dynamics

Keywords: CISS Effect, Magnetic Thin Films, NV Centers, Quantum Magnetometry

Long Time-Scale Magnetization Reorientation in Ferromagnetic Thin Films Induced by Chiral Molecules Adsorption

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Chiral molecules act as spin filters and spin polarizers for electrons passing through them. This phenomenon is known as the chiral induced spin selectivity (CISS) effect.1 Another aspect of the same effect, demonstrated magnetization reversal in a ferromagnet (FM) with perpendicular anisotropy after chemisorbing a chiral molecular monolayer without applying any current or external magnetic field.2 This phenomenon was observed when the easy axis of the FM was out of plane, and immediately after the adsorption process. This raises two questions: what effect does the easy axis have on the adsorption and magnetization reorientation, and, more importantly, is this effect due to the bonding event, held by the FM, or a long timescale effect stabilized by exchange interactions. We performed vectorial magnetic field measurements of the magnetization reorientation of a ferromagnetic thin film exhibiting perpendicular anisotropy due to CISS using nitrogen-vacancy (NV) centers in diamond, following the time dynamics of this effect. In parallel, we have measured the molecular monolayer tilt angle in order to find a correlation between the time dependence of the magnetization re-orientation and the change of the tilt angle of the molecular monolayer.3 Furthermore, the effects of the ferromagnetic easy axis direction on both the monolayer tilt angle and the magnetization reorientation of the magnetic substrate, were studied using magnetic atomic force microscopy (MFM),4 Results show that changes in the magnetization direction correspond to changes of the molecular monolayer tilt angle, and a clear correlation between the ferromagnetic layer easy axis direction and the tilt angle of the bonded molecules. providing evidence for a long-timescale characteristic of the induced magnetization reorientation. These results show that exchange interactions that are generated by the CISS effect can stabilize surface spins over long periods of time. The strong interaction between chiral molecules and FMs in static systems can pave the way for using the CISS effect in the fields of memory devices and spintronics.

Abstract ID: 901

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Non-destructive Inspection Techniques for Composite Materials and Structures

Keywords: acoustic emission, carbon fiber, polyamide, composite.

Acoustic emission at four-point bending of the carbon fiber – polyamide composite

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Plastics reinforced with carbon fibers are increasingly used in industries due to the unique combination of their elastic and strength properties with low specific gravity and chemical and corrosion resistance. They also have improved antifriction properties and relatively high surface conductivity, which in some cases can reduce the fire and explosion hazard of some production technologies. Nevertheless, the mechanical properties of such composite materials, especially under dynamic loading, require more careful study. Knowledge of the mechanical characteristics will allow starting the production of composites with specified parameters. Uvicom Co Ltd's samples of short carbon fiber polyamide thermoplastic produced by double screw extrusion were tested by four-point bending with linear load growth. Linear location of acoustic emission signals was carried out by two-channel acquisition system PCI-2 (PAC, USA). Investigation of the fractured samples surface by JSM-35 electron microscope (JEOL, Japan) showed that the predominant sources of acoustic emission were the ruptures of carbon fibers in the matrix. And only a few cases of the fiber-matrix adhesive contact disruptions were observed. Acoustic emission location data made it possible to trace the sequence of fracture nuclei development. It was also found that the total count and total energy release of acoustic emission events correlate with the volume of chaotically directed carbon fibers in the composite, which in our study was 10%, 15%, and 30%, respectively. On the base of alignment of our results with the data obtained through investigations of other materials fracture [1-3], a space-time model of the staged development of the process of material destruction is being developed.

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Abstract ID: 902

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Artificial photosynthesis

Keywords: Solar Fuel, Photocatalyst, Energy Conversion, CO2 reduction

Engineered Heterostructured Photocatalysts for Improved Solar to Chemical Fuel Generation

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Despite of extensive research being undertaken over the last few decades in designing photocatalysts, having maximum visible light absorption with appropriate band edge position for driving the H+/CO2 reduction reactions, the overall efficiency mainly governed by the charge carrier separation, stability, recyclability and overall cost are still nightmare to enthrust them in practical use. The photocatalysts which are relatively cost effective either suffer from stability (CdS, CdSe or Cu2O) and/or efficiency (Fe2O3, WO3, etc.), the solar to hydrogen generation efficiency (STH) lies below 1%.

One of the most crucial aspect that governs overall efficiency of the solar H2 generation and CO2 photo-reduction is charge carrier separation followed by the charge carrier transfer kinetics. In order to manipulate/tune these most intrigued elemental processes, we have designed heterostructured photocatalysts based on abundant elements, where the developed hetero-interface impart synergized properties such as improved charge carrier mobility, high absorption coefficient in the visible light and high dielectric permittivity (reduces the charge separation distance at the interface), arising from both, the counterparts.1-5 The detailed results on design of these heterostructured photocatalysts, their solar to chemical conversion efficiency and underlying change carrier dynamics will be discussed.

Abstract ID: 903

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Modulator, Defective metal-organic frameworks, Advanced oxidation technology, Persulfate, Sulfamethoxazole

Synthesis of modulated defective iron-based metal organic frameworks with enhanced catalyst performance for persulfate activation to effectively degrade Sulfamethoxazole in water

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Metal-organic frameworks (MOFs) materials have attracted widespread attention as a kind of advanced oxidation heterogeneous catalysts, which are commonly used for the efficient removal of emerging pollutants in wastewater. In this study, four novel defective iron-based Metal organic frameworks catalysts were successfully synthesized via a strategy by employing different modulators ((A) Formic acid, (B) Acetic acid, (C) Sodium acetate and (D) Ammonium acetate). The physical and chemical characterization illustrating that modulators could promote the formation of defects, specifically the existence of defects improve the crystallinity, promote Fe-O clusters coordination and enhance catalytic performance. The catalytic performance of Fe(II)-MOFs was detected through persulfate (PS) activation for degrading emerging pollutant sulfamethoxazole (SMX) in water. The defective Fe(II)-MOFs with modulator Formic acid exhibited excellent catalytic performance, it was found that the highest degradation efficiency for 0.039 mmol L-1 SMX was 92.63% in the conditions of the 1.0 g L-1 Fe(II)-MOFs-HCOOH dosage and SMX:PS 100:1. In addition, according to the chemical quenching, complete capture and EPR tests to confirmed that the reaction process was a free radical reaction dominated by SO4-• and •OH. The degradation pathways and mechanism of SMX in Fe(II)-MOFs-HCOOH /PS system reveal that defects generate coordinatively unsaturated metal sites and accelerate the transmission of electronic, which has important guiding significance for the application of defective MOFs in the treatment of emerging pollutants in wastewater.

Abstract ID: 905

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Solar Cells

Keywords: Dye-sensitized solar cells, titanium dioxide, photo-anode, hydrothermal

Synthesis of anatase-rutile mixed phase TiO2 photo-anode for dye-sensitized solar cells

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As a promising alternative to the conventional silicon-based solar cells, dye-sensitized solar cell (DSSC) has attracted intensive research interests over the past decades owing to its facile and low cost fabrication process compared to the silicon chip manufacture. Generally, a DSSC consists of transparent conducting oxide (TCO) substrate deposited with titanium dioxide (TiO2) film as photo-anode. Although the TiO2 photo-anode can be conveniently prepared by using the commercial TiO2 paste, there are several disadvantages about the commercial paste such as high cost and incapable of altering the TiO2 composition through doping for enhanced photovoltaic performance. Hydrothermal method is the most widely adopted technique for the synthesis of TiO2 photo-anode. Nevertheless, the reported processing steps for the hydrothermal synthesis of TiO2 photo-anode were intricate and thus complicated the overall DSSC processing. In this work, we have developed a reinvented methodology for the synthesis of anatase-rutile mixed phase TiO2 photo-anode by omitting several intermediate steps, which can simplify the whole DSSC processing significantly. By using the reinvented methodology, the DSSCs with promising photovoltaic performance were fabricated, which was comparable to the DSSCs based on commercial TiO2 paste. In addition, it was discovered that the rutile content in the TiO2 photo-anodes showed an increasing trend with prolonged hydrothermal durations. The improvement in DSSC efficiency with higher rutile content can be attributed to the synergistic effect between anatase and rutile phases in the DSSCs, in which the electron-hole recombination was inhibited by the electron transfer from rutile to anatase lattice trapping sites, thereby improving the photo-catalytic activity. This study offers a promising route to simplify the DSSC processing, as well as elucidating the influence of hydrothermal duration on the synthesis of TiO2 photo-anode.

Abstract ID: 906
Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)
Invited Talk
Topics: Point Defects, Doping and Extended Defects
Keywords: ZnO hybrid QDs, Blue emission, Frenkel defects, density functional theory

Blue Emissive ZnO Hybrid Quantum Dots

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Blue Emissive ZnO Hybrid Quantum Dots

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II-VI ZnO quantum dots (QDs) is one of the promising candidates to replace for blue light-emissive QDs containing expensive indium (In) or harzardous Cd- and Pb-elements. For developing blue emissive ZnO QDs, the removal of green, yellow emission known to be generated from oxygen vacancy defects is pre-requisite. Recently it was realized [1] that super-Eg excitation wavelength (λex) dependent Zni-V¬o complex defects related characteristic emissions of green, yellow, and orange-red from ZnO QDs were completely inhibited by reducing Vo's through the hybridization of Zni with antibonding O-states of graphene oxides (GO) QDs. Therefore, only blue emission from transition Frenkel pairs (Zni0-VZn) in ZnO-GO hybrid QDs was successfully achieved irrespective of λex and showed high photoluminescence quantum yield (PLQY) of 92%. In this study, another ZnO hybrid QDs are synthesized with hybridization of several ligands and of functionalized Acenes. Blue emission from these ZnO hybrid QDs is investigated and well explained by using photoluminescence, photoluminescence excitation (PLE), PL quantum yield, and density functional theory (DFT) calculation by comparing the electronic band structure.

Key Words: ZnO hybrid QDs, Blue emission, Frenkel defects, density functional theory

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Abstract ID: 907

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Sensors and MEMS: Materials and Devices

Keywords: volatile organic compounds, fluorinated, tin oxide, sensor, UV activation, transparent

An Innovative Approach to Photo-Chemiresistive Sensing Technology: Surface Fluorinated SnO2 for VOCs Detection

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Transparent electronics continues to revolutionize the way we perceive futuristic devices to be. In this work, we propose a technologically advanced VOC (volatile organic compound) sensor in the form of a thin film transparent display fabricated using fluorinated SnO2 films. A solution-processed method for surface fluorination of SnO2 films using SelectfluorTM as a fluorinating agent has been developed. The doped fluorine was optimized to be < 1% resulting in a significant increase in conductivity and reduction in persistent photoconductivity accompanied by a faster decay of the photogenerated charge carriers. A combination of these modified properties, together with the intrinsic sensing ability of SnO2, was exploited in designing a transparent display sensor for ppm level detection of VOCs at an operating temperature of merely 150 °C. Even a transparent metal mesh heater is integrated with the sensor for ease of operation, portability, and less power usage. A sensor-reset method is devised while shortening the UV exposure time, enabling complete sensor recovery even at lesser operating temperatures. The sensor is tested towards a variety of polar and non-polar VOCs (amines, alcohols, carbonyls, alkanes, halo-alkanes, and esters), and it exhibits an easily differentiable response with the sensitivity falling in-line with the electron-donating tendency of the functional group present. This work opens up the door for multiplexed sensor arrays with the ability to detect and analyze multiple VOCs with specificity.

Abstract ID: 908

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Functional Magnetic Materials

Keywords: Magnetic Thin Film, Magnetic Domain, Inclined Easy Axis, Domain transition

Functional property of adjacent narrow thin film strips with inclined uniaxial magnetic anisotropy

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A magnetic momentum in a magnetic thin film behaves as if it is restricted in a 2-D sheet, due to the strong demagnetizing force along the thickness direction of the film. The momentum in the film clustered by the exchange force and forms a certain pattern of magnetic domain. A formation and variation of the pattern of magnetic domain is dominated by magnetic energy which is affected by the external field, the anisotropy energy, and the 2-D shape of the film. In this study, we utilize the quasi-2D property of magnetic thin film to a functional device such as a sensor having a memory function or a switched device using it's specific magnetic phenomenon.

Our previous research shows that a narrow rectangular shaped thin film element with inclined in-plane easy axis in 70 degrees has a typical characteristic of magnetic domain transition. The transition phenomenon also can be controlled by a normal magnetic field. In this report, we apply this controlling method to parallel line adjacent many-body configuration of elements having the typical transition property in each element. There is mutual magnetic interaction existing within the many-body elements. A high frequency permeability as a function of the domain transition of the many-body element is also investigated. It is important for realizing a high-density device using this phenomenon.

Abstract ID: 909

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Photonic devices and applications

Keywords: Polyanilines, Conductive Magnetic Nanocomposites, Superparamagnetic Fe3O4, Polymer Solar Cells.

Application of superparamagnetic nonocomposites from polyaniline derivatives and Fe3O4 in optoelectronic devices (solar cells)

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Polyaniline (PANI) is a very popular conducting polymer because of its easy synthesis, low-cost monomer, high stability, its adjustable characteristics comparing other conducting polymers and its countless usage in different industries is interesting [1]. The electronic industry is one of the industries in which PANI has many applications in making solar cells [2-6]. The magnetic field and/or mixing magnetic nanoparticles can be used in the solar cell structure for increasing the lifetime of the exciton [2-6]. We showed that using magnetic nanomaterials in the active layer of the solar cells is an effective factor for increasing the efficiency of solar cells by producing local magnetic fields in creating the spin-orbit coupling which can increase the triplet state relative to the singlet state [2-6].

In this lecture, I wish to report a summary of our recent works on the application of the novel superparamagnetic core-shell nanocomposites of PANI derivatives and Fe3O4 nanoparticles. The most important innovation in this type of nanocomposites is the in-situ production of superparamagnetic Fe3O4 nanoparticles simultaneously with the polymerization of PANIs in solid-state. The main point is the use of FeCl3.6H2O as both an oxidant and the source of Fe3 + ions, which is reduced to Fe2+ after oxidation of the aniline monomer and initiation of the polymerization process. Then, the core (Fe3O4) -shell (PANIs) structure is produced by adding sodium hydroxide solution (NaOH/H2O) in work up to the simultaneous presence of Fe2+ and Fe3+ in the resulting solid mixture.

It can be confirmed by different mechanisms such as a spin-orbit coupling and singlet fission (SF), which can increase the triplet state of excitons and/or trimerons formation. The other factor influencing the source of this great success is the presence of covalently grafted -SO3H groups in PABS on the surface of TiO2 in addition to core-shell morphology.

These novel devices display major advancements in the field of polymer solar cells for energy conversion based on the high performance of simple, stable, and single-layer cells with low-cost fabrication materials, and facile and green preparation method for both nanocomposite and cell. It is concluded that such cells offer a promising new approach to commerce the new solid-state polymer solar cells.

Abstract ID: 910
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Dielectric, Ferroelectric and Piezoelectric materials
Keywords: Nanospring CNT, Nano composites, P(VDF-TrFE), dielectric constant

Highly Dispersible Buckled Nanospring Carbon Nanotubes for Polymer Nano Composites

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Highly Dispersible Buckled Nanospring Carbon Nanotubes for

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II- We propose the unique structure of highly dispersible single-walled carbon nanotubes (SWCNTs) in various solvents and polymers using the ZnO nano particle template. Buckled nanospring-shaped carbon nanotubes (NS-CNTs) were synthesized by a chemical reaction of ZnO nanoparticles with acid-treated SWCNTs and then dissolving ZnO through chemical etching. The unique structure of distorted hexagonal NS-CNTs encircled around ZnO nanoparticles was formed by the bending of SWCNTs caused by the agglomeration of chemically adsorbed Zn(OH)2, which is further crystallized as the polycrystalline ZnO inner core. The highly dispersible NS-CNTs could be incorporated in the poly[(vinylidenefuoride-co-trifuoroethylene] [P(VDF-TrFE)] copolymer, one of widely studied ferro-and piezo-electric polymer, up to the value of 15 wt% as nanofllers. The relative dielectric constant (K)

of polymer nanocomposite, at 1 kHz, was greatly enhanced from 12.7 to the value of 62.5 at 11 wt% of NS-CNTs, corresponding to a 492% increase compared to that of pristine P(VDF-TrFE) with only a small dielectric loss tangent (D) of 0.1.

Key Words: Nanospring CNT, Nano composites, P(VDF-TrFE), dielectric constant

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Abstract ID: 911

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Superconductivity and Superfluidity

Keywords: Topological Superconductivity, Weyl semimetals

Topological Superconductivity in Sr¬ intercalated Bi2Se3 and its implications for quantum computation

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Topological Superconductivity in Sr¬ intercalated Bi2Se3 and its implications for quantum computation

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The discovery of Dirac and Weyl semimetals (WSM) has brought forth the condensed matter realization of Dirac/Weyl fermions, which were previously theorized as low energy excitations in high energy particle physics. In the recent past we have witnessed some exceptional developments in chalcogenide and pnictide materials that have been identified with such properties. The age-old industrial thermoelectric materials based on selenides and tellurides have been turned into topological insulators and Weyl semi-metals. Superconductivity derived from such exotic systems promises to usher-in new understanding of correlated electronic systems. In this talk we shall review electromagnetic properties of topological superconductor Sr-intercalated Bi2Se3 and study its pairing mechanism by muon spin rotation measurements. A brief discussion on current trends in realizing quantum computers by using properties of topological superconductors will be included. Furthermore, several transition metal mono-pnictides are under intense investigation for understanding properties of inversion-symmetry broken Weyl semimetals. Non-trivial Berry phase and chirality are important markers for characterizing topological aspects of Weyl semimetals. We shall discuss aspects of exceptional magneto-resistance seen in the normal state of these topological semimetals.

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Abstract ID: 912

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Gas sensors, Reduced graphene oxide, swift heavy ions

Role of multi-step reduced graphene oxide for gas sensing applications

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Application of reduce graphene oxide for gas sensing is one of the most fascinating applications. They are operable at room temperature unlike metal oxide based conventional sensors. Furthermore, the properties like high specific surface area, light weightness, make them suitable candidate for gas sensing applications. The response is stable under ambient conditions. We used a novel multistep reduction method (1) based upon swift heavy ion irradiation to synthesize reduced graphene oxide (rGO) from graphene oxide (GO) (2). The first step is to reduce GO by hydrazine hydrate followed by irradiation of the sample by swift heavy ions (SHI) of Ag^8+ at different ion fluences ranging from 10^11 to 10^13 ions/ cm^2. It was evident from the Raman spectra of the irradiated samples that the surface amorphorization increases with irradiation. We have designed a sensor to sense sulfur dioxide at the concentration levels as low as 5ppm. The pore surface area of the sensing samples increases with swift heavy ion treatment. The oxygen functional groups contribute to the selective binding interaction to different gas molecules. The observed sensing response of rGO may be due to increase in number of defects as well as increase in its microporous structure, which results into better diffusion of gas molecules driven be capillary forces. The increased porosity and higher surface to volume ratio resulted in higher adsorption and desorption of the chemical species. The maximum sensing response of 7.35% was observed at 5ppm of SO2 The response is also selective to this analyte. The gas sensing response is further attributed to electron transfer between rGO and the analyte gas.

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Abstract ID: 913

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Photonic devices and applications

Keywords: Fluorescent sensor, open aperture Z scan, Nonlinear optical absorption, Excited state absorption, optical limiting

Third Order Optical Nonlinearity of Styrylcyanine Based Fluorescent Sensor

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Third Order Optical Nonlinearity of Styrylcyanine Based Fluorescent Sensor

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Fluorescent compounds with large stoke shifts and tunable wavelength broadly studied for device application such as sensing technology, biomedical imaging and key component of optoelectronic devices. Organic compounds with delocalized π electrons have significant application in optical limiting and optical switches. We report the third order optical nonlinearity of the styrylcyanine based fluorescent sensor, (E)-2-(2-(3, 3-dimethyl-3H-indol-2-yl) vinyl)-4-nitrophenol [1]. UV-Vis absorption and Photoluminescence spectra of the compound studied in Diacetone alcohol and it shows good stock shift. The nonlinear optical studies were carried out by using a single beam Z-scan technique [2], which uses an exciting source of laser pulse having 7ns pulse width at 532nm. The open aperture Z scan signature of the sample studied at different input beam intensities and the valley shaped curves symmetric about the focus indicate the presence of nonlinear absorption and optical limiting properties (Fig.1). The sample shows decrease in nonlinear optical absorption with increase in input intensity (Fig.2) and is due to the combined effect of two photon absorption and excited state absorption [3]. The investigated light emitting nonlinear material is a potential candidate to act as a good optical limiter.

Fig.1: Open aperture Z Scan data Fig.2: Variation effective two photon absorption coefficient with I0

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Abstract ID: 914

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Fiber reinforced Composites

Keywords: Textile Reinforced Concrete (TRC), Carbon fiber, Glass fiber, Galvanized iron fiber, Drop weight test

Dynamic Behavior of Carbon, Galvanized Iron and Glass Textile Reinforced Concrete Subjected to Impact Loading

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Textile Reinforced Concrete (TRC) has already shown much development as a light weight and thin-walled structural element with high load bearing capacity by evaluating its performance against static loading. Because of its high tensile strength properties, TRCs can be suitable to resist impact loading. Therefore, objective of this research is to investigate the dynamic behavior of TRC under impact loading and to present a comparison of performance between carbon fiber (CF), square oriented galvanized iron fiber (SGIF), diagonal oriented galvanized iron fiber (DGIF) and glass fiber (GF) as textile reinforcement with concrete. Performance of TRC with CF (8 mm opening); SGIF (4 mm opening); DGIF (6 mm opening) and GF (4 mm opening) are evaluated by drop weight impact test method recommended by ACI-544 committee. Total 18 TRC plates of size 300 x 170 mm2 and thickness of 25 mm (DGIF and GF), 50 mm and 75 mm (GIF and CF) were tested by dropping an impact load of 4.49 kg from a height of 457 mm with the help of a hardened steel ball of 63.5mm diameter. The number of impact blows at initial crack and ultimate crack were counted and the velocity of the impact load is measured with the help of a high-resolution camera. Performance of the samples is compared by the dynamic and static impact energy. Because of the smaller opening of the fiber fabrics, maximum aggregate size was selected to be 2.36 mm. GI short fiber (0.5% of cement weight) with 0.51mm diameter and 36 mm long was used in concrete. Firstly, 3 TRC plates of DGIF and GF reinforced TRC each (25mm thickness, 1-layer reinforcement) were tested and DGIF textiles showed better results than GF textiles; although the overall performance of both were not satisfactory. Next, SGIF having high tensile properties was taken to compare with another high-performance CF textile. Total 12 TRC plates of 2-layer reinforcement, 3 for each combination (thickness and reinforcement) were tested. For 50 mm and 75 mm thick plates the dynamic and static impact energy of CF is more than 2 times and 1.25 times greater respectively than the TRC with SGIF. Therefore, against impact loading, CF textiles are proved to be the most suitable textile reinforcement; however, SGIF textiles can be an alternative option for CF textiles.

Abstract ID: 915

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Particulate reinforced Composites

Keywords: Thermal conductivity, polyester, heat dissipation, Silicon Carbide, Boron Nitride

Thermal interface management in digital electronics with multi-modal inorganic and organic fillers and coupling agents in polymer composites

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This research work basically throws light on the next generation of materials which possess excellent thermal and mechanical stability for thermal interface materials in digital-electronics. As we know that during the operation of digital-electronics, there is entrapment of heat due to denser concentration of integrated circuits in a relatively compact space, there are chances of failure due to thermal coupling between the circuits. Therefore, it is very essential to allow the heat to be dissipated and removed from the circuits for trouble free operation. Again, digital electronic components tend to have very low toughness and impact strength. So, organic filler having good mechanical properties can be used as a reinforcement to improve the strength of the composites owing to higher life and lower failure rates. Inorganic fillers like Silicon Carbide and Boron nitride particulates of various sizes and shapes and an organic filler i.e. peanut husk were chosen for the present investigation in polyester matrix to fabricate thermally improved polymer composites. In addition to that, silane and titanate were used as coupling agents for the surface modification of fillers. In hybrid composites, the network formations between the fillers become more because of structuring of fillers with high aspect ratios. The larger particles along with comparatively smaller treated particles showed a highly improved thermal conductivity due to larger surface contact as well as better adhesion and hence higher connectivity pathways due to percolation. The surface modification also results in composites exhibiting a low coefficient of thermal expansion compared to the non-modified ones. Thus, a new composite material was proposed with improved strength and thermally conducting but electrically insulating properties which can be used as substrates and packaging materials in digital electronics.

Abstract ID: 916

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Topological Insulators, 2D Materials, and Voltage Controlled Magnetism

Keywords: Topological insulator, BSTS, transport

Studying the Hall effect and magnetotransport properties of planar structures and microstructures of topological insulators Bi1.08Sb0.9Sn0.02Te2S and Bi1.04V0.04Sn0.02Sb0.9Te2S

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Topological insulator is an insulator whose inner bulk is ordinary zone insulator but there are topologically protected gapless conducting electrons on the surface. Such exotic materials are of particular interest because they are promising both for fundamental and applied researches. Nowadays doped compounds Bi1.1Sb0.9Te2S (BSTS) [1, 2] are considered the most perspective.

We carried out transport measurements of micro bridges (~10 um) created with Focused Ion Beam (FIB) and macro samples (~1mm). The T-dependency of conductivity shows that with the temperature decreases at high temperatures (> 100 K) the conductivity increases exponentially typically for insulators and at low temperatures (< 100 K) linearly falls typically for metals which can be explained by the surface conductivity of topological insulators. Additionally, we placed the samples in high magnetic field (up to 16 T) perpendicular to their plane and observed Shubnikov-de-Haas (SdH) oscillations at higher fields and behavior specific for weak anti-localization and localization in the neighborhood of 0 T. The Hall effect was also observed in the experiments, and the H-dependency of Rxy was extremely nonlinear. SdH effect allowed us to evaluate the charge carrier density which was in good compliance with Hall measurements (n_2DEG≈3.6·〖10〗^12 см^(-2)). Using the Hikami-Larkin-Nagaoka theory we could evaluate the T-dependencies of scattering time and length of charge carriers.

Abstract ID: 917

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Fiber reinforced Composites

Keywords: Silica aerogel, aerogel-fiber composite, hydrophobicity, nano titanium dioxide, IR opacification, thermal insulation, ASTM C335.

Role of in-situ formed TiO2 nanoparticles on high temperature thermal insulation efficiency of hydrophobized silica aerogel-E glass fiber composite studied by horizontal heat pipe test set up (ASTM C335) at steady state.

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Fiber reinforced silica aerogel composites / blankets have proven to be good thermal insulation. Their thermal performances have been reported in the literature in terms of thermal conductivity. However, there has not been much information available on thermal performance of these composites at high temperatures, especially at actual conditions of the applications. Considering, industrial pipe insulation application, the hydrophilic silica aerogel-Eglass fiber blanket (B1) was hydrophobized (B2) using silica precursor MTMS (MethyltrimethoxySilane) via co-precursor method and then IR opacified (B3) using in-situ prepared nano titania (using TIP (Titanium tetraisopropoxide)) to improve thermal performance. Since, TiO2 demonstrates the best IR scattering properties below 8µm [1], TiO2 is chosen as IR opacifier in this study. The effect of hydrophobization and IR opacification of hydrophilic composite on thermal performance is studied using horizontal heat pipe apparatus developed using ASTM C335 at steady state. The hydrophobization using silica precursor has increased the surface temperature of the composite at all operating temperatures (from 100°C to 600°C). This is due to the increased solid conduction with increase in silica content. The addition of small fraction (2 wt%) of in-situ prepared nano titania to this hydrophobized composite, had reduced the surface temperature at every operating temperature to almost near to the unmodified silica aerogel blanket.

Abstract ID: 918
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Green Composites
Keywords: Key Words: Pillared Clay, Metal Poly-cation, Adsorption

Optimization of Pillared Clays for Adsorption Applications in Aqueous Solutions

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Optimization of Pillared Clays for Adsorption Applications in Aqueous Solutions

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Clays are eco-friendly, porous, high surface area materials which may also be transformed into an effective adsorbent. It contains exchangeable cations and also hydroxyl functional groups on its edges and hence it may serve as an efficient adsorbent for organic species as well as metal cations. However, untreated clay swells upon contact with water. Due to this problem the use of clay in tall adsorbents towers becomes a challenging task. This problem may be easily resolved through pillaring of the clay. Pillared clays prepared by intercalation of single and mixed metal polycations are being actively explored. The clays reparation may proceed through the conventional as well as process intensified route using ultrasound treatment.

In this study, the effect of different process variables including frequency of ultrasound, time for the formation of polycations, and intercalation time was studied in a systematic manner using the Design of Experiment approach. The prepared samples were analyzed for Cation Exchange Capacity [CEC], surface area, and point of zero charge [PHZC]. Further characterizations were carried out using FTIR, XRD, TGA, SEM, EDAX, and NMR. The pillared clays samples were optimized for the adsorption of metal ions and organic dyes. The results revealed that the adsorbent was of higher quality than the ones conventionally prepared in literature. Optimization studies on the processing conditions of the preparation of pillared clays were done. Adsorption studies with different cations and dyes were also studied and the corresponding optimization for the best-pillared clays for each of the pollutants was done.

Abstract ID: 919

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Ferroelectricity and piezoelectricity

Keywords: Ferroelectric polymers, ultrathin substrate, imperceptible, energy harvesting, ultraflexible organic diodes

Imperceptible energy harvesting device and biomedical sensor based on ultraflexible ferroelectric transducers and organic diodes

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Energy autonomy and conformability are essential elements in the next generation of wearable and flexible electronics for healthcare, robotics and cyber-physical systems. This study presents ferroelectric polymer transducers and organic diodes for imperceptible sensing and energy harvesting systems, which are integrated on ultrathin (1-µm) substrates, thus imparting them with excellent flexibility. It was found that these ultraflexible ferroelectric polymer transducers (UFPTs) develop improved ferroelectric properties through thermal annealing resulting in an increased crystallinity. After poling the remnant polarization reaches values up to 70 mC/m^2 in close correlation with the crystallinity and the decrease of the dielectric constant. Simulations show that the sensitivity of ultraflexible ferroelectric polymer transducers can be strongly enhanced by the use of the ultrathin substrate. The ultrathin substrate furthermore allows the mounting of the transducers on 3D-shaped objects and the stacking in multiple layers. Indeed, UFPTs have improved sensitivity to strain and pressure as compared to devices on rigid thick substrates with values up to 15 nC/N; they have a fast response (<< 20 ms/N) and an excellent mechanical stability with a bending radius down to 40µm. Accordingly, they can be used as imperceptible wireless e-health patches for precise pulse and blood pressure monitoring. For harvesting biomechanical energy, the transducers are combined with full wave organic rectifier circuits made of ultraflexible organic diodes. These diodes are based on organic thin film transistors with short-circuited drain and gate and are fabricated on the ultrathin substrate as well. The diodes have an excellent on/off ratio up 107 and a transition voltage around 0V. Transducers, diodes and ultrathin capacitors (needed as storage elements) were further combined to form an imperceptible, 2.5 µm thin, energy harvesting device with an excellent peak power density of 3 mW/cm^−3.

Abstract ID: 920
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Multifunctional composites
Keywords: Fireworks, Green crackers, Functional additives

Multifunctional Composite Additives for Reduced Emission Fireworks

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Fireworks are a low explosive pyrotechnic device that uses combustion and explosion to produce an illumination or auditory effect for aesthetic and entertainment purposes.

The celebration of national, traditional and cultural events with fireworks is standard practice across the globe. The bursting of fireworks often generates dense smoke of particulate matter (PM) and gaseous emission in the environment, which ultimately degrades the air quality. Emissions from firecrackers have potential health hazards, and the development of reduced emission firework is still challenging to pyrotechnicians. Our group developed four proprietary additives with functionalities that are presently not there in conventional firecrackers.

The functional additives are zeolite and iron (III) oxide (Fe2O3) with functionalities of i) providing dust suppressants on fragmentation ii) absorbing gaseous emissions, iii) arresting release of particulate matter, iv) sorbing or sequestering metal, v) releasing oxygen and negative ions. The additives are functionalized by functional molecule like shellac to improve stability and functionality. These additives have been used in sound and light-emitting firecrackers with potassium nitrate (KNO3) as an oxidizer. The usage of functional additives in firecrackers composition give promising emissions reduction more than 30% for particulate matter (PM10 and PM2.5) compared with firecrackers without functional additives (conventional firecrackers). The functional additives increase the activation energy of flash powder by virtue of thermite reaction without compromising the performance of firecrackers.

Abstract ID: 922

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Sandwich materials/hybrids, Multifunctional composite, Advanced composites

Keywords: Infrared Detectors, Perovskite Films, Quantum Dots

Study of Hybrid Infrared Detectors with Perovskite Films and Quantum Dots

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The material class of perovskites has become a rising star in the optoelectronic applications. Over the very recent years it has demonstrated an astonishing growth of the power-conversion-efficiency in perovskite solar cells (more than 20%). Besides solar cells, perovskite photodetectors also achieved eye-catching results in the past five years. In the case of the visible light great detectivity, microwatt/mm2 illumination level detection, and nanosecond response speed have already been achieved. However, the processes in the field of near-infrared (NIR) wavelength range are still under investigation. We developed hybridized device containing quasi-2D perovskite with cadmium sulfide quantum dots (QDs) for NIR sensitive structure. It was successfully integrated with the silicon substrate. Two different patterns of the electrode materials (comb-shaped and narrow stripped) were realized by gold DC sputtering and photolithography. For the samples the spectral response, responsivity to different exposure source intensities, detectivity (normalized and angular) and response times were studied. This paper offers a promising route to optimize the performance and the electro-optical properties of the novel perovskite materials and their hybrids, and paves the path for developing high-performance electrode patterns suitable for infrared detection purposes.

Abstract ID: 923
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Smart Composites
Keywords: Shape memory polymer composites, grabbing systems, space sustainability

Shape Memory Polymer Composites: Smart Materials for Space Sustainability

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Shape memory polymer composites (SMPC) are a new class of smart materials. They have typical properties of composites and in addition shape memory properties. In fact, they can change their configuration reacting to specific external stimulus, mostly heat-induced, and remember the original shape. Considering the low weight, the stiffness and strength, the possible shape reconfiguration, and recovery force, the SMPCs are very interesting for space applications and sustainability. In fact, they are expected to be used as self-deployable structures (e.g., solar sails) or as grabbing systems of space debris (see Fig.1).

To evaluate their behaviour on Earth, in microgravity and the harsh space environment, a series of experiments have been carried out. This study provides an overview of such experiments for developing functional materials for new space applications. Moreover, the new concept of space sustainability is deepened and the importance of such functional materials exploited for future space colonization.

Abstract ID: 924
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Carbon and metal oxide based composite materials
Keywords: nanodiamond, surface chemistry

Fine control of detonation nanodiamond surface chemistry towards functional materials

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Nanodiamonds (NDs) behave suitable chemical and physical properties for a wide range of applications in medical, energy or quantum domains. Detonation synthesis provides a mass production technique of well-controlled NDs, with a primary size of ca. 5 nm. However, a shell made of various surface terminations as well as graphitic or disordered carbon surrounds the diamond-core after the synthesis. The fine control of this superficial chemistry is essential to understand and take advantage of the interfacial and semi-conducting properties of NDs. For instance, a hydrogenated surface provides a negative electron affinity to the nanodiamond, which is deeply investigated to use them as a solid source of solvated electrons in water. On the opposite, an oxidized surface promotes the colloidal stability of NDs in different polar solvents, which is of great interest for the synthesis of nanocomposite.

This contribution will focus on the studies conducted in our group to better control NDs surface chemistries using thermal and microwave plasma treatments. The complementary combination of characterization techniques we used all over the years will be presented. Then, we will describe some applications in which surface chemistry plays a crucial role and directly drive the behavior of our nanomaterial, such as its incorporation in polymeric composite.

Abstract ID: 925

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Processing and manufacturing technologies

Keywords: Additive Manufacturing, Knee implant, Polymer, Biomedical, Mechanical Strength, Wear

Evaluating the mechanical strength of the articulate component fabricated using the additive manufacturing process in the biomedical application

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Additive manufacturing is a layer by layer production technique which has been applied for different applications such as aerospace, automotive and biomedical application. In the biomedical field, especially the demand for knee implants is increasing worldwide due to arthritis problems. Furthermore, patient-specific implants are required because they will serve the patient reliably for a longer duration. The articulating component made up of polyethylene, attached to the femoral and tibial section experiences the most wear and bears the maximum load. Earlier, these components are developed by using the traditional technique like investment casting but lack structural integrity. Therefore, there is a need to fabricate the articulating components using a new technique like (FFF) Fused Filament Fabrication process, which allows us to increase the mechanical strength of the product by varying the process parameters such as layer thickness, infill density, printing speed and part orientation. The mechanical strength of the samples is evaluated by analyzing the compressive strength, wear-resistance, and fatigue strength of the polymer. The optimum parameters of the FFF process are selected based on the analysis and applied to the fabrication of the prototype (articulating component)

Abstract ID: 927

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster Presentation

Topics: Photonic devices and applications

Keywords: Core-shell NPs, silver nanoparticles, chlorobenzene, z-scan, Ag@C

Nonlinear optical properties of Ag@C metal@organic core-shell nanoparticles.

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Recently, nanocomposites made of noble metal nanoparticles with graphene and its other allotropes are getting much consideration owing to its enhanced linear and nonlinear optical properties [1]. In this direction Ag@C core-shell NPs were prepared using the laser ablation of Ag plate in Chlorobenzene using an Nd:YAG laser operating at a wavelength of 532nm [2]. The third order nonlinear optical measurements for Ag@C core-shell nanoparticles and ablated Chlorobenzene were conducted using an open and closed aperture Z-scan experiment(fig.1). Ag ablated in chlorobenzene shows good optical limiting (fig.2). Reverse saturable Absorption behavior is observed in open aperture Z-scan and Nonlinear refraction effects were negligible. Characterization was done using UV-VIS spectroscopy and gives similar results for both Ag@C and ablated chlorobenzene. SPR peak corresponding to Ag NPs is suppressed due to formation of graphite shell around Ag NPs.

Abstract ID: 928

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Electrical properties of graphene, Mxenes and other two-dimensional materials

Keywords: Graphene, Carbon Nanotube, Molecular Sensors, Electronic transport

Electronic transport and molecular adsorptions of graphene and CNT layers for designing molecular sensors by first-principles study

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Molecular/chemical sensors are needed in many fields of environmental monitoring, medical diagnosis, etc. To detect molecules, electronic sensors based on field effect transistors (FETs) are often employed. In those sensors, the changes of the conductance in the FETs induced by the adsorption of the targeted molecules are utilized for the detection of the molecules. However, it is difficult to selectively detect the targeted molecules among various molecules. In this talk, I will report the adsorption effects of environmentally polluting and/or toxic molecules on the stability and the electronic transport of graphene layers and carbon nanotube (CNT) layers, based on our first-principles density-functional study [1-3]. It is shown that only NO and NO2 molecules can strongly bind with boron-doped graphene layers in air, and therefore the electrical conductivity can be dramatically changed by the adsorption of those molecules. Furthermore, it is shown that toxic CO molecule is selectively detectable by using the anisotropic behavior of the electronic transport of the CNT layer. These results would provide highly important information for designing molecular sensors with high selectivity and sensitivity.

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Abstract ID: 929

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Superconducting and magnetic materials

Keywords: Crystal structure, XRD

Crystal structure study of BaPbO3

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BaPbO3 is a simple perovskite which forms the base compound from which several superconductors have been synthesized. Despite having attracted much attention due to its interesting physical properties, the driving mechanism behind the BaPbO3's metallic behaviour have been poorly understood. There are contradicting reports about the crystal structure of BaPbO3. Additionally, despite the compound being metallic[1,2], the density of states at fermi level are very low[3]. To understand this, we have studied the evolution of the crystal structure with temperature of BaPbO3 using high resolution x-ray diffraction (XRD). Rietveld analysis of the XRD data suggests that BaPbO3 is an orthorhombically distorted perovskite that crystalizes in the Ibmm space group at all temperatures ranging from 300K to 10K. We also report the change in the behaviour of the lattice parameters below 150K that are not merely due to thermal effects. The resistivity data reported in the literature[4], combined with our crystal structure study suggests that there might be a link between the electronic behaviour and the crystal structure. Further analysis are in progress in order to understand this unique electronic behaviour of BaPbO3. We believe that our study will be helpful in understanding the origin of superconductivity when doped with bismuth and other elements like strontium.

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Abstract ID: 930

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Solar Cells

Keywords: Perovskite Solar Cells, Organic Solar Cells, Nanoscale Structure-Function Relationships

Nanoscale Function in Perovskite and Organic Solar Cells

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Perovskite and organic solar cells are promising for enabling low-cost solar energy harvesting, while offering a lightweight and flexible form factor. Despite stunningly rapid progress in the performance of organic-inorganic lead halide perovskite solar cells, the causes of local spatial heterogeneities in photovoltaic properties remain poorly understood. For organic solar cells, the nanostructured interpenetrating donor-acceptor active layer required for high performance operation poses a challenge for disentangling the effects of nanoscale structure on optoelectronic processes. In this talk, I will outline our recent efforts to unravel nanoscale structure-function links in these emerging photovoltaic systems. Using point-by-point current-voltage mapping based on conductive atomic force microscopy [1], we observed an enhanced open-circuit voltage and suppressed short-circuit current near grain boundaries in methylammonium lead halide perovskite active layers. Nanoscale nonlinear strain and surface potential mapping provide evidence for field-induced methylammonium cation buildup and band bending near grain boundaries that reduce charge carrier recombination, but may trap charge [2,3]. Nanoscale point-by-point current-voltage mapping of hole mobility in bulk heterojunction organic solar cells highlights the importance of in-plane charge transport pathways for facilitating out-of-plane charge flow [4,5]. This conclusion is bolstered by data that shows improved charge percolation when there is balance of crystallite orientations. These experiments highlight the significant role of nanoscale structure in emerging photovoltaic systems and the importance of co-localized nanoscale structure-function analysis to unlock the potential of new photovoltaic materials.

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Abstract ID: 931
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Porous and cellular materials
Keywords: EBM porous structures, Ti6Al4V, TiN coating, gas nitriding, bipolar plate, fuel cells, corrosion

Development of TiN coatings by gas nitriding on AM Ti-6Al-4V open cell porous structures for PEMFC bipolar plates

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Proton-exchange membrane fuel cells (PEMFC) development includes the goal of Bipolar plates (BP) weight reduction since this component represents from 50-80% of total weight of the stack and Ti presents itself as a great candidate for this application. However, Ti passivation takes place during the operation of the PEMFC reducing the ability of the BP to transport electrons between cells. Among the different solutions proposed for increasing surface conductive properties and corrosion resistance on Ti-6Al-4V, TiN coatings obtained by gas nitriding method represent an excellent route, due to its good conductivity combined with corrosion resistance. Moreover, BP based on porous materials are gaining interest to replace conventional flow-channeled BP due to improvements in the distribution of reactants and products. For this purpose, additive manufacturing (AM) techniques such as Electron Beam Melting (EBM), allow the production of open-cell structures with controlled features. TiN coating combined with the porous structure produced by AM are high potential technologies that have not been covered in BP development together and, consequently, there are no studies regarding the enhanced effect of both aforementioned state-of-the-art technologies.

The present work studies the development of TiN coating by gas nitriding on Ti-6Al-4V open structures produced by EBM, and their effect on the corrosion behavior and the interfacial contact resistance.

Abstract ID: 932

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Zinc ferrite nanoparticles, Structural properties, Dielectric properties, Gas sensing properties

NH3 Gas Sensing Properties of ZnxFe3−xO4 (x = 0 and 0.5) Nanoparticles Synthesized by Sol-Gel Auto-Combustion Method

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Now-a-days iron oxide nanoparticles have been used to develop tunable filters and optical switches those work under magnetic fields, absorbants, sensors, catalysts, coating, and insulating aerogels [1-2]. In recent years, preparation and properties of transition metal doped spinel ferrites with the molecular formula MxFe3−xO4 (M = Zn, Cu, Ni, Mn, Co, etc.) have been widely studied towards the development of opto-electronic devices [3-5]. Among these spinel ferrites, semiconductor zinc ferrite have drawn a lot of attention due to its potential applications in gas sensor, semiconductor photocatalysis, magnetic data storage, ferrofluid, medical imaging [3-5]. The properties are also depends upon the particle size and synthesis conditions. In the present work, ZnxFe3−xO4 (x = 0 and 0.5) nanoparticles are synthesized by sol-gel auto-combustion method. The samples are annealed at 200, 400 and 5000C temperatures for 6 h. The influence of annealing temperature on composition and morphology of ZnxFe3−xO4 (x = 0 and 0.5) are investigated by XRD and FESEM. For x = 0, with the increase in annealing temperature, the transition from Fe3O4 (magnetite, cubic) to α-Fe2O3 (hematite, rhombohedral) phase is observed. It confirms that with the Zn doping the cubic spinel structure of host nanoparticles remains unaffected with the variation in annealing temperature. With the doping of Zn in iron oxide, the reduction in the crystallite size and band gap is observed for Zn0.5Fe2.5O4 as compared to that of pure iron oxide nanoparticles. Furthermore, frequency dependent parameters like dielectric constant, dielectric loss, ac conductivity, and electric modulus is measured for all the samples. Possible sensing mechanism of undoped and Zn doped iron oxide nanoparticles is studied towards NH3 gas. The improved response of the Zinc doped iron oxide nanoparticles towards ammonia gas is found as compared to that of undoped iron oxide nanoparticles, exhibiting their potential for application in nanosensors.

Abstract ID: 934

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Ceramic based composites

Keywords: Ultra high temperature ceramics, Spark Plasma Sintering, Oxidation

Effect of Silicon Carbide Size on Oxidation Behavior of ZrB2

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ZrB2 is a member of ultra-high temperature ceramics which has find its application in space vehicles. In this respect, the oxidation behaviour during its interaction with the environment becomes important to study. Several reinforcements have been added to to improve its oxidation resistance and SiC is one of the most promising one pertaining to the formation of protective SiO2 layer. In the current study, ZrB2 incorporated with SiC of two different particle sizes (D50 ~ 30 µm and ~5 µm) to form two composites of same composition (ZrB2-20 vol. % SiC) but different reinforcement size, was processed using spark plasma sintering. Higher densification of ~ 98 % was obtained for fine SiC reinforced composite while as a densification of ~ 89 was achieved in coarse SiC reinforced composite. To investigate the oxidation behaviour, specimens from each composite (10 × 3.6 × 5 mm3) were tested at 1500 °C for 3 hours in air. It was observed that with coarse SiC, oxygen influx was easier through less dense composite resulting in the formation of thicker oxide layer of SiO2 on the top (~ 9-94 µm thick), In the case of fine SiC reinforced composite, thinner oxide layers (silica layer of ~ 4 µm) were formed. Thus, finer SiC shows higher resistance to oxidation, however, for longer durations thicker scale of SiO2 in coarse SiC composite would also provide protection from further oxidation unless the operating temperature exceeds the vaporization temperature of SiO2.

Abstract ID: 935

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: Perovskites, photoluminescence, low-dimensional materials

Colloidal Low-dimensional perovskite: synthetic strategies and optical properties

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Perovskite materials have emerged as very promising materials for optoelectronic, photovoltaic, and more recently photocatalysis due to their outstanding optical and electronic properties. Lead halide perovskite (LHP) responds to the general formula APbX3, where A is an organic cation such as methylammonium, formamidinium, or inorganic cation such as Cs+, and X is a halide anion (Cl-, Br- or I-). LHP can be prepared with different stoichiometries and morphologies: low dimensional material such as 1D nanowires/nanorods, 2D nanosheets/nanoplatelets, and 0D nanoparticles. The first colloidal dispersion of lead bromide perovskite nanoparticles (CH3NH3PbBr3) was synthesized using long ammonium salts as organic ligands, resulting in a good luminescence quantum yield (20 %) and stability in a battery of low polar solvents. The preparation of few-layered perovskites with the formula L2[APbX3]n−1PbX4, where L represents the ligands and n corresponds to the number of PbX6 perovskite layers sandwiched between organic ligands layers have received great attention. They exhibit strong quantum confinement due to their thinness and present very narrow absorption and emission peaks with small Stokes-shift. According to the nature of the organic ligands and the synthetic methodology, we were able to prepare two-layered [APbBr3]PbBr4 perovskite nanoplatelets with blue-deep emission and good chemical/photochemical stability. Moreover, novel colloidal nanocomposites were obtained in the presence of cycloalkylammonium bromide, lead polymer, and perovskite nanocrystals leading to long, 1D well-defined architectures.

The key role of the organic ligands for surface passivation, the dimension of colloidal perovskite establishment, and the preparation of novel heterostructures together with a general overview of the colloidal perovskite applications will be discussed.

Abstract ID: 936

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Nanogenerators and self-powered nanosystems

Keywords: Hybrid Nanomaterials, Smart Textiles & Devices, Energy Storage, Energy Harvesting

Hybrid Smart Textiles and Devices for Energy Harvesting & Storage: Nanotechnology in Motion towards Self-Powered Technologies

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The ever-growing progress of the emerging market of wearable electronics has been driving the need for advanced all-in-one energy harvesting & storage technologies integrated on clothing for several applications ranging from Healthcare and Sports to Fashion and Defense. Thermoelectric energy harvesting technology is a promising solution for wearables since it convert the low-grade waste heat from ubiquitous thermal energy sources into electrical energy. Supercapacitors are a clean and safe energy storage solution to produce wearable energy storage clothing, owing to their high power density, fast charging, long cycle life and robustness.

The combination of both technologies in a single ALL-IN-ONE device opens new horizons towards the next generation of self-powered flexible/wearable electronics.1

Nanotechnology and Nanomaterials fostered innovation in the Textile and Clothing industry, to impart new functionalities on fabrics while preserving their comfort and lightness properties.

In this talk, we will provide an overview of our recent achievements in the design of smart textiles and devices for energy applications, from supercapacitor devices towards an innovative all-in-one self-powered energy harvesting & storage technology.2-4 The journey from the concept and design of advanced functional nanomaterials, their incorporation on textile and flexible plastic substrates and assemble of hybrid multi-tasking systems will be presented.

Key Words: Hybrid Nanomaterials, Smart Textiles & Devices, Energy Storage, Energy Harvesting

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Abstract ID: 937

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Electrochemical Supercapacitors

Keywords: Electrochemical capacitors, Transition metal dichalcogenides, Carbon materials, Aqueous electrolytes, Organic electrolytes

Carbon/ReS2 composites as an attractive electrode materials in electrochemical capacitors

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Electrochemical capacitors (ECs) show to be a promising filling between fast response, high power density conventional capacitors and high energy density metal-ion batteries (MIBs). While employing carbon-based materials satisfies the demand for high power density ECs, providing high energy density without deteriorating power capabilities is challenging. Considering the energy density equation, researchers are dedicating their efforts to enhance the energy density of ECs through two different approaches: first, an integration of conductive carbonaceous components with redox-active materials such as metal oxides, hydroxides or sulphides which enhance the specific capacitance of ECs. Especially, transition metal dichalcogenides (TMDs) are placed at the centre of attention in ECs design due to the incorporation of sulphur atoms instead of oxygen, which offers higher conductivity. Second, extending the working voltage of ECs through utilizing non-aqueous electrolytes to eliminate hydrogen and oxygen evolution reactions as the result of water decomposition is proposed. TMDs are represented by the formula of MX2, where M is a metal atom (Mo, V, Re, etc.) and X is a chalcogen atom (S, Se or Te). Recently, ReS2 has gained significant attention due to attractive electrical, optical and vibrational properties. Additionally, its exhibit unique distorted 1T structure which gives the in-plane anisotropy in the fundamental physical properties [1]. ReS2 is most commonly exploited in MIBs due to large interlayer spacing of 6.14 Å. The capacitor application is rarely described [2]. In this study, ReS2 composites were prepared with different carbon materials such as three-dimensional graphene-like (3DG), carbon nanotubes or graphene nanoplatelets by hydrothermal reactions. Various structural/textural properties of these composites were characterized by scanning electron microscopy, X-ray diffraction or Raman spectroscopy. The electrochemical performance were evaluated by cyclic voltammetry, galvanostatic charge/discharge and impedance spectroscopy. Two- and three-electrode cells were employed for testing carbon/ReS2 composites with aqueous and organic electrolytes.

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Key Words: Electrochemical capacitors, Transition metal dichalcogenides, Carbon materials, Aqueous electrolytes, Organic electrolytes

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Abstract ID: 938

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Functional Magnetic Materials

Keywords: Metal oxide, Spinels, Superparamagnetism, Nanostructures

Inducing room temperature Superparamagnetism in iron, manganese and cobalt oxide Spinel nanostructures by Nickel incorporation

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Inducing room temperature Superparamagnetism in iron, manganese and cobalt oxide Spinel nanostructures by Nickel incorporation

First row transition metal oxides with spinel structure are interesting materials due to their excellent magnetic and catalytic properties, which have also been utilized as electrode materials in energy storage devices.1 Although most of these metal oxides have antiferromagnetic behavior, substitution with other transition metal ions transforms them to ferromagnetic. Due to inherent ferrimagnetic nature and multivalent metal ion constitution, these metal oxide nanostructures are highly attractive for heterogeneous catalysis. However, inducing superparamagnetism at room temperature would make them even attractive for biomedical applications such as in magneto-hyperthermia.2 Magnetic behavior of a metal oxide is defined by its lattice spin arrangement, which in turn, depends on its composition.3 In this talk, we will present the results of structural and magnetic characterization of some metal oxide nanostructures of spinel structure (NixFe3-xO4, NixCo3-xO4 and NixMn3-xO4) to demonstrate the possibility of inducing superparamagnetism in them through Ni incorporation. Based on structural analysis, we propose reasonable cation distributions in the binary metal oxides nanostructures that can explain their observed magnetic behaviors. We also demonstrate that a phase transition from antiferromagnetism to superparamagnetism can be induced in these nanostructures by incorporating a certain amount (mol fraction) of nickel ions in their lattice. Induction of room temperature superparamagtism in these metal oxide nanostructures is the result of the combination of two factors: (i) the strong preference of Ni2+ ions to occupy the octahedral sites of the spinel lattice, and (ii) smaller effective magnetic moment of the Ni2+ ions compared with Co2+/3+, Mn2+/3+ and Fe2+/3+ ions. Octahedral site preference energy (OSPE) of the ions in the lattice is a key parameter to explain these results.

Key Words: Spinels, Superparamagnetism, Nanostructures.

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Abstract ID: 939

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: Electrochemical capacitor, Biomass-derived carbon, Soft-template method, Frequency response

High frequency response of biomass-derived carbon in aqueous electrochemical capacitor

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Electrochemical capacitors are the devices for reversible energy storage. They are characterized by high power output owing to non-faradaic type of charge storage, while having only limited energy density. This parameter is governed by both capacitance (C) and cell voltage (U). The cell voltage is essentially dependent on the specific electrolyte type (aqueous, organic, ionic liquid), while the capacitance is mainly influenced by the active surface area of carbon. However, it has been already shown that additional contribution to the capacitance is achieved thanks to the pseudocapacitance originated from heteroatoms present in the electrode material, mainly nitrogen, but other, like sulfur, oxygen and phosphorus are also reported.

In this work, we demonstrate the high capacitance of biomass-derived carbon based on nitrogen-rich adenine precursor obtained via soft-templating method. The performance of two-electrode system (with 1 mol L-1 Li2SO4 electrolyte) equipped with a reference electrode is compared to the commercially available carbon Kuraray YP-50F. The interesting parameters of the carbon is not only the superior gravimetric capacitance comparing to commercial carbon (100 F g-1 vs. 130 F g-1), but also the outstanding frequency response shown in Fig. 1. The extensive studies aiming at the correlation of physicochemical properties of these carbons with electrochemical performance will be provided.

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Abstract ID: 940

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanomaterials and Nanotechnology

Keywords: Astrocytes, graphene, organic semiconductor, biopolymers, glial interfaces

Glial interfaces: biomaterials, devices and approaches to trigger and monitor the "other brain".

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Evidence produced over the past 30 years showed crucial roles of glial cells, called astrocytes, in brain function and dysfunction and moved the neurocentric vision of brain science towards a mole holistic perspective. Since astrogliotic reactivity is a major cause of failure of brain implant performance, the study of astrocytes/material interaction can also drive knowledge on engineering safe and long-term stable biosensors and bioelectronic neural interfaces.

A major pitfall in the study of astrocytes is that technologies used to understand their mechanism, structure and function are limited or adapted from those engineered for neuronal cells. In this context, the goal of our study is to validate bioelectronic materials, devices and biophotonic approaches to selectively probing and sensing astrocytes physiology (namely ion channels, water channels and calcium signalling) and to understand their role in brain physiology and pathology. In this respect, the presentation will overview the results obtained on: 1)using of bioelectronic devices, based on silicon nanowire, graphene and organic semiconductor, that allows stimulation and recording of astrocytes calcium signalling and voltage membrane oscillations, 2)the potential of photonic and optical approaches to trigger selective calcium signalling in astroglial cells 3) the use of nanostructured interfaces that allow for generating a model of astrocytes in vitro mimicking morphological structure and function they show in-vivo.

The presented results evidenced that glial interfaces might help in unveiling unexpected role of astrocytes in brain cognitive function and can provide novel path for therapeutical neuromodulation approaches.

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Key Words: Astrocytes, graphene, organic semiconductor, biopolymers, glial interfaces

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Abstract ID: 941

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Concrete and cementitious composites

Keywords: Biochar, sustainable concrete, sulphate, chloride, durability.

Effects of silica rich biochar on cement mortar hydration kinetics and durability under chloride and sulfate environment

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This study investigated influence of biochar, prepared from rice husk and waste wood, on hydration kinetics and resistance to chloride and sulfate attack of cementitious composite.

The resistance in terms of strength retention, mass change, expansion and micro-structural changes was studied and compared to similar properties of mortar under normal wet curing.

Findings suggest that rice husk biochar (RHB) contain 15–16% amorphous silica, although its carbon content (42%) and specific surface area are significantly lower than wood biochar (79% carbon and surface area of 227 m2/g). Both types of biochar at 1 wt% dosage increase rate of hydration at early stage than control, attributed to high surface area, finer size than cement and nucleation of cement hydrates on biochar surface. Both RHB and MWBC at 1–2 wt% significantly reduce water permeability than control, which is also reflected in 15–18% improvement in strength at 7-day, 42-day and 120-day age of cement mortar. Lower permeability due to addition of both biochar types reduces rate of mass gain due to sodium chloride absorption, contributing to 9% higher strength than control after 120-day exposure period. Based on strength, water-cement ratio and cement content, the tested mortars are suitable for exposure class of XS2 (EN 206), where the concrete is always submerged in water. When exposed to sodium sulfate solution, 1 wt% of RHB and 1 wt% of MWBC are found to improve strength by 14–17 % than control after 120-day, while minimizing loss in strength due to sulfate attack. Micro-structural analysis shows pore blocking action of biochar mitigates micro-structural damage due to sulfate attack. This offer higher dimensional stability, reflected from 62 to 68% less expansion of MWBC-mortar and RHB-mortar compared to control. These findings suggest suitability of biochar-mortar application under moderate sulfate environment.

Abstract ID: 942

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Low dimensional, nano and 2D materials for optical devices, Flexible Electronics, Sensors & Composites

Keywords: 2D perovskites, light emission, phonons, excitons, Raman spectroscopy, quantum wells

2D Perovskites for Color-Tunable Light Emission

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Two-dimensional metal halide perovskites are novel materials that have attracted great interest for the development of next-generation optoelectronic devices due to their outstanding figures of merit in photovoltaic solar cells, and in light-emitting devices, which come along with high defect tolerance, low-cost solution processing and tunable emission across the visible spectrum. They consist of atomically this alternating organic and inorganic layers, and this highly anisotropic architecture provides unique elastic, dielectric, and optoelectronic properties that lead to peculiar phenomena, such as self-trapping of excitons due to local lattice distortions. Furthermore, the strong confinement of the charge carriers in the inorganic layers makes such structures natural quantum wells that are appealing for fundamental research and photonic applications. Recently, our group demonstrated how the choice of the type of organic molecules can be exploited to engineer the optical properties of these 2D materials.1-4 Here we deepen this approach by a systematic study of their photophysics and vibrational properties at room and cryogenic temperature. The self-trapped exciton emission strongly depends on the organic cation type and temperature. Similarly, the rich spectrum of vibrational resonances is governed by the organics that determine the distortions of the single octahedra layers.

Abstract ID: 943
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Bio-composites
Keywords: nanoparticle, liposome, cochlear, cell culture, gene, cochlear implant

Liposome nanoparticle as a potential vehicle targeting inner ear cells for rehabilitation of hearing function---cultured inner ear cells used for nanoparticle biocompatibility test and histochemical localized genes as assumed targets.

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Profound sensorineural hearing loss (SNHL) is one of the most common diseases that have no effective treatment. Among the causes of SNHL, including advanced age, ototoxicity and noise exposure, gene mutation constitutes a cause leading to a substantial number of children with hearing loss that generally needs a cochlear implant (CI) for rehabilitation of the hearing. Integrating vehicles at nanoscale to CI was explored hoping to make it a way to improve CI function. Genetic SNHL is irreversible and some responsible genes can even worsen the hearing during adulthood. We checked the expression location of some of such genes in normal hearing cochleae specimens. Nanoparticles are tested in guinea pig inner ear cell culture for the purpose of obtaining information how the cochlear neurons and other cells interact with the nanoparticles, e.g., nanoparticle internalization and toxicity. The nanoparticle of liposome are internalized into the cultured neurons as well as glial cells without visible toxic effects by the nanoparticles on the cultured inner ear cells. The nanoparticles with reliable biocompatibility can serve as a vehicle for biomaterial delivery into inner ear compartments where targets are often isolated by barriers, such as blood-labyrinthine barrier. Using CI electrodes, routes across the round/oval window and injection into endolymphatic fluid for delivering the nanoparticles into the cochlea are discussed. Possible payloads (peptides, drugs, genes that help protect or even reverse hearing damage) and in vivo researches are reviewed.

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Abstract ID: 944

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Manufacturing and formation techniques

Keywords: Chalcogenides, Thermoelectric, Energy Storage, Spark Plasma Sintering

Enhancement of thermoelectric properties of Bismuth sulfide by Hallide Substitution

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Over the past few decades, semiconducting chalcogenides compounds (A2B3 with A = Sb, Bi, As and B = S, Se, Te) receivedlot of attentionsfor thermoelectric applications. Among these chalcogenides sulphides-based (Bi2S3, Cu2-xS, CdS, TiS2, Ag2S etc.)compounds have the advantage ofhaving low cost, low toxic, more abundant elements. However their ZT values need to be improved. Various strategies such as doping have been used for improving its TE performance. Here, we report the synthesis and thermoelectric properties of Bi2S3doped with CaCl2synthesized by spark plasma sintering. XRD of all the samples show single phase formation. All the compositions exhibit a negative Seebeck coefficient suggesting n-type behavior. The increasing dopant concentration leads to the improvement in its electrical property. As a result, higher power factor ~700μW/m-K2has been achieved in these composites, which is by much higher than the maximum power factor ever reported in the literature for Bi2S3 based compositions. Further electron transport and heat transport mechanisms have been evaluated in co-relation with FESEM, XPS and TEM.

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Abstract ID: 945

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Shape-memory alloy

Keywords: Lever arm, Force, Compliance, Stiffness, Superelastic SMA wire

Compliance Control by Structural Modification for Effective Force Handling using Superelastic SMA Wire

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Recent progression in research in the field of medical robotics is towards smart material based compliant mechanisms and structures that involve appropriate actuator designs to exhibit actuation forces for robotic motion or to stimulate human muscles/joints. A sensing mechanism to detect the force exerted by these actuators is required; this article focuses on the design and development of a force sensing prototype engaging flexible, passive superelastic (SE) SMA wire in a compliant lever arm architecture. The superelastic wire attached at the effort arm of the lever exhibits easier deflection for load at the load arm and the resistance change of the wire gives the measure of the input load. A compliant controlled robotic arm that enables structural modification through the repositioning of the pivot for the sensed force is fabricated and analyzed. The force handling capability of the robot is enhanced using stiffness control which is accomplished by the structural alteration corresponding to the input force. The stiffness control is achieved by the position control of the pivot of the lever arm mechanism.

The material used for the assembly is a lightweight aluminium, the geometrical dimensions of the elements for the sensing/actuating mechanism are designed based on the technical features of the device. The proposed mechanism features a manipulator arm (load arm) capable to pick up several millinewtons of force. When the input force pushes the lever, the end effector (effort arm) experiences greater deformation if this point is farther from the fulcrum, while it undergoes lesser deformation when it is nearer the fulcrum. The pivot is positioned initially near the load arm; on adding mass at the load arm, the deflection caused at the effort arm due to force is detected by the resistance variation of the SE wire. The adaptive stiffness behaviour of the lever designed for the force applied makes the system compliant. The compliance of this actuating assembly is fixed and the position of the pivot is determined by the load; thus, the physical compliance is unchanged. The assembly uses a dynamic structural mechanism based on the load that helps to maintain the compliance of the robot. The prototype is designed and constructed using a class one lever architecture inclusive of the sensor mechanism is tested where the stiffness of the structure is varied to a constant value as per the weight at the load arm to experience compliant actuation for the input force. The amplified actuator requires no power, produces larger constant stroke and compliance.

Abstract ID: 946

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster/Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: Electrochemical capacitors, Ageing, Carbon electrodes, Aqueous electrolytes, Energy Storage, High Power Device, Floating

Novel exploitation protocols for capacitor lifetime enhancement

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Sustainable energy storage devices like aqueous-based electrochemical capacitors (ECs) are intensively sought to ensure the novel technologies are clean, eco-friendly and cost-effective. However, water-based systems have not been successfully commercialized so far, while organic-based devices are already available on the market. To diminish negative aspects of strongly acidic or alkaline electrolytes (corrosion, safety), pH-neutral electrolytic solutions have been proposed; their environmental aspect and high hydrogen and oxygen evolution overpotentials allow the capacitor voltage to be exceeded far above theoretical water splitting (1.23 V). Lithium nitrate (LiNO3) aqueous solution was proposed as a promising candidate for electrolyte in carbon-carbon symmetrical ECs. In one of our previous studies, the electrochemical performance of capacitors operating with 1 mol L-1 LiNO3 aqueous solution was investigated upon different voltage loadings (from 1.3 up to 2.0 V), and the origin of system fade (C/C0=80% and ESR increase by 100%) was determined [1]. Mostly, two aging mechanisms were discussed accordingly to the voltage applied, with a value of 1.5 V as a discriminant between them. Positive electrode has been oxidized, and a deposit (e.g., Li2CO3) has been found on both electrodes after long-term floating tests. Nonetheless, the specific surface area (SSA) of the negative electrode is not remarkably affected by the aging process; the electrochemical hydrogen sorption is assumed to etch the electrode surface that might help to maintain high SSA, despite Li2CO3 precipitation.

In our next-step study, we propose advanced floating protocols as an alternative way for LiNO3-based capacitor lifetime enhancement. Two optimization pathways are proposed (alternate and reversed floating) to exploit both electrodes' features fully.

This approach has been verified using different nitrate concentrations: 0.2, 0.5, 1 and 5 mol L-1. Successful lifetime enhancement was achieved, up to +83% time prolongation (210 vs. 384 h of EC floating test with 0.2 mol L-1 LiNO3).

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Abstract ID: 947

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: : Reduction, adsorption, Graphene oxide, Metal doped Graphene oxide, Methylene blue, metal-lic sulfide NP

Transitional metal sulfide nanoparticle doped graphene oxide: Synthesis, characterization, and photocatalytic reduction of methylene blue to leuco methylene blue in aqueous mixture

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The graphite (Gt) was functionalized to gra-phene oxide (GO) through a green route in a highly controlled oxidation process using non-explosive oxidizing mixture at 55o C in high yield. The GO was doped with NiS, ZnS, and CdS transitianl metal sulfide nanoparticles (TMS NPs) in 1:1 ratio respectively at 85oC. TMS NPs were obtained by using chloride salts of Ni, Zn, and Cd metals with thiourea in 1:3 ratio in aqueous GO dispersion for in situ dop-ing. The GO and TMS NPs doped GO (TMSNP-GO) were characterized with X-ray diffraction (XRD), FTIR, UV-Vis spectropho-tometry, Raman spectroscopy and thermograv-imetric analysis (TGA). The GO, NiS-GO, ZnS-GO and CdS-GO had photocatalyzed the meth-ylene blue (MB) reduction by 88%, 79.68%, 89.87% and 97% to leuco MB (LMB) colorless, in aqueous medium (Figure 1). Contrary to NiS-GO, the CdS-GO and ZnS-GO both had increased MB reduction by 9 and 1.87% respec-tively by weakening intersheet van der Waals forces of GO for availing surface area. The Ni2+ with 3d8 catalyzed 10.19 and 17.32% less MB to LMB than Zn2+ with 3d10 and Cd2+ with 4d10 elcterons respectively. MSNPs were uniformly doped with 2D GO sheets through a sulfide anion (S2-) releasing activity for a higher reduc-tion from water and electronically active sol-vents. MSNP-GO-MB-LMB ventures a novel host-guest chemistry as the MB with sp2 along with sp2-sp3 hybridizations of GO are photo-catalyzed to LMB. MSNP-GO-MB-LMB for-mulates a multifunctional nanocluster to ab-sorb solar energy and heat contents due to MSNPs-GO interfaces. Likewise ethylene (EB) and propylene blue (PB) could be separated through selective reductions as per their hydro-phobicity.

Abstract ID: 948

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: water splitting, bandgap, amorphous SiC

Bandgap engineering of amorphous sputtered hydrogenated silicon carbide thin films for photoelectrochemical water splitting

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Bandgap engineering of undoped and Al doped sputtered amorphous hydrogenated silicon carbide (a-SiC:H) thin films was carried out to assess light absorption properties of the material by maintaining the silicon to carbon stoichiometry without compromising its photoelectrochemical water splitting capabilities. Properties tailoring was achieved by varying the hydrogen concentration in the semiconductor during the deposition process and trough post-deposition thermal treatments. Optical constants were retrieved by suitable methods for the accurate determination of the fundamental absorption of dielectric thin films. Bandgap values were obtained by fitting the fundamental absorption using three different models, namely iso-absorption, Tauc and Band-fluctuations. Variations in the structure and hydrogen composition were tracked by Infrared and Raman spectroscopy techniques. Differences among bandgap values extracted by the distinct methods and their correlation to a-SiC:H structural features demonstrated that a structural disorder, rather than a hydrogen rearrangement or depletion, would be responsible for the observed annealing induced optical bandgap enhancement. The tuning of the optical bandgap of the p-doped a-SiC:H sample, with low hydrogen concentration, showed a gradual increase of the bandgap from 2.59 to 2.76 eV. The latter increase was induced upon the annealing steps from 200 °C till 600 °C. After heating at 600 oC the electric performance was strongly improved and required ohmic contacts were obtained. These bandgap values are close to the reported minimum bandgap necessary for water splitting taking into account overpotentials. We believe that these results will contribute to the design of monolithic tandem solar cells for water splitting applications.

Abstract ID: 949

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Polymeric composites

Keywords: 3D printing, biomaterial, dentistry, high-performance polymers, medicine, patient-specific implants

PEEK- A high-performance polymer used as patient-specific implants

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PEEK (polyetheretherketone) which is a high-performance polymer has great potential as using patient-specific implants in the field of medicine and dentistry because of its biocompatible properties. Recently, patient-specific implants are common due to their best fitting components with the anatomical structures. In addition, patient-specific implants fabricated from PEEK are common in the field of plastic surgery applications. On the other hand, the intraoral applications of PEEK are rare and limited to intraoral implant-supported prostheses. PEEK implants or frameworks are fabricated by subtractive technologies. However, patient-specific implants should fit the anatomy. Therefore, patient-specific implants require complex design which should be fabricated by additive manufacturing known as 3D printing.

In this report, the possible applications of patient-specific implants fabricated from 3D-printed PEEK will be discussed with rare case reports and treatment outcomes as well as finite-element analysis reports. Material properties as well as future applications of PEEK –a high-performance polymer- will be introduced.

Abstract ID: 950

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Transparent Conductors

Keywords: ITO, Tb, luminescence, energy transfer

Luminescence activation of terbium doped indium tin oxide and its impact on the host's optical and electrical properties

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The effect of terbium doping on the electrical, optical, and light emission properties of sputtered indium tin oxide thin films was investigated. The films were prepared by radio frequency dual magnetron sputtering maintaining a high optical transmittance in the ultraviolet and visible spectral regions and an electrical resistivity ranging from of 5×10-3 to 0.3 Ω-cm. Terbium-related luminescence is achieved after thermal treatments in air at 470 °C at atmospheric pressure. Electrical resistivity and optical transmittance were registered after each annealing step to evaluate the compromise between the achieved light emission intensity, electrical and optical properties. Additionally, Tb-related luminescence thermal quenching is assessed by temperature-dependent photoluminescence measurements, from -190 °C to 300 °C, under non-resonant excitation. Thermal quenching activation energies suggest an effective energy transfer mechanism from the ITO host to the rare-earth ions. This indirect excitation mechanism is tentatively modeled using a spherical potential well, as well as a tight-binding one-band approximation, approach for a short-range charge trapping process and subsequent formation of bound excitons to rare-earth ions clusters.

Abstract ID: 951

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Anodes and cathodes Materials

Keywords: 2D materials, rGO, Li Ion battery, anode materials

Nanocomposite 2D material matrix for battery anode materials

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Porous $CoFe_2O_4$ nanoclusters with different concentrations of graphene based composites were synthesized by a simple solvothermal process. The electrochemical properties of prepared $CoFe_2O_4$–reduced graphene oxide (rGO) composites were evaluated using polyvinylidene fluoride and Na-alginate as binder materials.

The synthesized porous $CoFe_2O_4$–rGO composites were characterized using an X-ray diffractometer (XRD, X'pert PRO MPD, PANalytical, Philips) with Cu Kα radiation (λ = 1.54 Å at 40 kV and 30 mA). The size and shape of synthesized samples were examined using Field Emission Scanning Electron Microscopy (FESEM)-EDS (JSM-7600F, JEOL). Transmission electron microscopy with energy dispersive spectroscopy (TEM), JEOL 2010F HRTEM, Japan, with 200 kV operating voltage was used to capture the morphology and crystallinity of porous $CoFe_2O_4$–rGO composite samples. The $CoFe_2O_4$ + 20% rGO composites with alginate binders deliver a stable maximum discharge capacity of 1040 mA h g−1 at 0.1 C, which is nearer to the theoretical capacity (914 mA h g−1) of this material. The alginate binders hold the integrity of the electrode and 20% rGO will give the electron transportation network during the conversion reaction in $CoFe_2O_4$ + 20% rGO composites/alginate electrodes.

Abstract ID: 952

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Transparent Conductors

Keywords: Indium tin oxide, ITO, charge carrier density, band gap energy

Optical and electrical properties analysis of sputtered tin-doped indium oxide thin films taking into account growth induced inhomogeneities

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Indium tin oxide (ITO) layers were prepared by radio frequency magnetron sputtering on fused silica substrates at low substrate temperatures in order to induce and assess the variation of the optoelectronic properties by post annealing treatments in an argon atmosphere. These layers show a growth induced inhomogeneous microstructure, which impacts the optoelectronic properties of the system [1]. The lowest resistivity measured by four-point probes obtained in this work was 2.5×10-4 Ω.cm after heating in argon at 500°C. Optical transmittance, elemental composition and electrical resistivity measurements were performed after each annealing step. In this work charge carrier density and carrier mobility were monitor after each annealing temperature by an optical analysis in which the films are treated as a two layers stack with different Drude parameters. Additionally, the intrinsic band-gap, Burstein Moss shift and valence effective mass are determined [2]. It was found that the optical band-gap energy increases with increasing carrier density for carrier densities above a critical value. Optical parameters such as refractive index, absorption coefficient, and band gap were estimated accordingly at each annealing temperature.

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Abstract ID: 953
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Polymeric composites
Keywords: Composites, Membrane, Halloysite Nanotubes, Polyaniline

Composite polymer membranes for electro-devices and their transport properties

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Polymer electrolyte membranes (PEM) are widely used as promising material in the electrocatalyst devices. We produced a novel type of composite single- and two-layer PEMs with multifunctional properties based on MF-4SC polymer (Russian analogue of Nafion) modified by pristine halloysite nanotubes and nanotubes coated by polyaniline. Hybrid bi-layer PEMs demonstrate an apparent asymmetry of transport properties depending on their orientation to the counterion flux in the electrochemical cell. By systematically investigation of electrical conductivity, diffusion permeability, current-voltage curves, it is found that the inclusion of polyaniline into PEMs leads to minor decreasing of diffusion permeability, preservation and even strengthening of electrical conductivity, and constant value of the limiting electrodiffusion current density in contrast to the pristine PEM. The comparison of two methods for the bilayer membrane formation (casting and airbrushing) shows that the layering increases the porous structure of the PEMs. This study offers a potential opportunity to improve the diffusion permeability and asymmetry of transport properties by choosing ratio of the layer's thicknesses and modifier percentage for the manufacturing of PEMs to be applied as solid polyelectrolyte films in fuel cells and other electrical devices.

Abstract ID: 954

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Solar Cells

Keywords: silicon, nanowires, doping

Advanced doping techniques for nanostructured solar cells

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Silicon based solar cells have represented the leading actors in the last decades photovoltaic market share with respect to all the other technologies, thanks to the Si abundance, stability and non-toxicity, and future projections confirm this predominance also in the years to come. However, half of the cell module cost is due to the material used and to its processing. In order to decrease the costs, it is known that a cut in the Si consumption must be operated. This will decrement the optical absorption and consequently the output generated current. To keep the performance level, a large number of special Si surface designs aimed at light harvesting have been proposed. One of the most popular approaches is to use silicon nanowires embedded in the solar cell emitter as optically and electrically active layer. Thanks to their excellent optical properties they have represented the first choice for many academic approaches. In this context conventional doping methods have shown limitations, not yet overcome despite the technological developments, such as use of expensive equipments and materials, need of numerous steps to obtain conformality, formation of structural defects or precipitates and limited control on ultra-shallow diffusion depth. Recently an alternative doping process has been proposed, the molecular monolayer doping (MD) [Nat Mat 7 (2008) 62, Mater Sci Eng B 178 (2013)686, Phys Stat Sol A 212(8) (2015)1685, Mat Sci Semic Proc 42 (2015)200, Appl Mater Interf 8 (2016)4101]. MD provides conformality, does not introduce structural defects, does not use dangerous and expensive sources or equipments and allows to control the junction depth at nanometer level. The process is based on the self-assembling of a molecular monolayer of specific dopant precursors on the Si substrate. Then an annealing step releases the dopant atoms from the monolayer and diffuse them into the substrate. Thanks to the source self-assembling mechanism the dopant atoms density and positions are determined, depending on the molecule steric properties. With MD is possible to achieve junction depths as small as 5 nm and to fabricate FETs and solar cells [Nanoletters 9(2) (2009) 725, Sol En Mat & Sol Cells 132 (2014)118]. The talk will provide a brief overview on the morphological, chemical and physical properties of the assembled molecules, focusing on the characteristics of the molecule/Si interface which plays a strategic role on the electrical performance of the final samples. New results on the dynamics of the molecule modification during the self-assembling and the thermal process, from the chemical and morphological point of view will be also presented. The results of the integration of the molecular doping on silicon nanowires will be shown and discussed, together with the electrical results obtained on the solar cells where the Si nanowires have been integrated as emitters.

Abstract ID: 955
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Nanocomposites
Keywords: Mxene, Soot oxidation, Transition Metal Oxides

Mxene and TMO (Transition Metal Oxides) Composites for Soot Oxidation Application

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Catalytic soot oxidation is a complex process occurring on the gas-solid-solid interface of the reacting gas, catalyst, and soot surface. It is highly dependent on the presence of surface-active sites such as oxygen species. Pt, Rh and other noble metals have been used as a catalyst but are limited due to its high cost. As an alternative, earlier our group has reported thermally stable hydrogen annealed HfO2 and sustainable bi-metal doped clay material.1,2 In this study, we are proposing a two-dimensional transition metal carbide popularly, Mxene for use as a catalyst. Mxene has been explored for various applications in the field of energy storage, biomedical applications, and clean-up technologies.3 The proposed topic studies the use of Mxene and its composites with TMO as a support for catalytic oxidation of soot. The inherent network system and good porosity of the Mxene can be used for incorporating catalytically active species and will act as an excellent pathway for migration of active species for rapid soot oxidation. The current study explores yet another diverse application of Mxene based materials and will play a significant role in industrial scaling up for technologies used in soot oxidation catalysts.

Abstract ID: 956

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: Borophene, Electronics, Finite Element, PEDOT:PSS, Polymer Nanocomposite

Thermal Conductivity and Thermomechanical properties of Borophene /PEDOT:PSS nanocomposite: A Numerical Study.

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The highly electrical conducting organic material- Poly(3,4-ethylene dioxythiophene): poly(styrene sulfonate) PEDOT:PSS, has found application in cutting edge devices such as in rechargeable batteries and electrochemical capacitors. However, such electrode is known to fail due to thermal strain and mechanical stresses induced during lithiation. Besides, the performance of such material is often adversely impacted by temperature variation. To address this limitation, PEDOT:PSS is often reinforced with highly conductive nanofillers such as Xenes, Xanes and MXenes having superior electrochemical and mechanical properties. Therefore, in this study, we aim to investigate the thermal conductivity and temperature dependent properties of Borophene /PEDOT:PSS nanocomposite using numerical studies.

Abstract ID: 957

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Graphene, Mxenes and other two-dimensional materials for biomedical and healthcare applications

Keywords: Water-Soluble Fullerene Derivatives, Antiviral Properties

Design of water-soluble fullerene derivatives with promising antiviral properties

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Viral infections are responsible for 90% of human infectious pathologies. Efficiency of the existing antiviral drugs is limited by their narrow action spectra, development of drug-resistant viral strains and toxicity effects. Therefore, there is an urgent need for the development of new types of antivirals with improved performance. Water-soluble fullerene derivatives demonstrated extremely promising antiviral properties against HIV, CMV, HSV, Hepatitis C, Influenza, and Stomatitis and Ebola viruses in some cases overcoming efficiency of commercial drugs. Importantly, several fullerene derivatives inhibit simultaneously more than one viral target, thus suppressing significantly the formation of drug resistance.

Recently we reported efficient and selective methods for the synthesis of a broad range of water-soluble fullerene derivatives [1-3], which substantially decreased costs of these compounds and made them available in bulk quantities for biological studies. We will discuss four new synthetic routes for conversion of readily available C60Cl6 and C70Cl8 precursors to a variety of stable water-soluble fullerene derivatives bearing up to 16 carboxylic groups in their molecular frameworks. Several fullerene derivatives revealed low toxicity in combination with a pronounced activity against Influenza, HIV, CMV, and HSV, which makes them promising compounds for the development of novel antiviral drugs.

Key Words: Water-Soluble Fullerene Derivatives, Antiviral Properties

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Abstract ID: 958

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Potassium Ion Batteries

Keywords: Potassium-Ion Batteries, Energy Storage

Organic redox-active materials for high-capacity and high-rate potassium-ion batteries

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Using organic redox-active molecules provides a new paradigm for future development of metal-ion batteries. Indeed, organic materials are usually based on light elements (C, H, N, O, S) and, therefore, can enable much higher specific capacities compared to the salts and oxides of heavy transition metals. Most of organic materials are non-toxic and environment friendly, which makes easy their recycling as a common household waste. In contrast to crystalline inorganic cathodes and anodes, organic materials are soft and, therefore, can operate at high charge and discharge rates thus leading to design of ultrafast batteries. Mechanical properties of polymeric cathodes and anodes enable their application in truly bendable batteries for emerging generation of portable electronics.

Lithium-ion batteries currently represent one of the mainstream energy storage technologies. However, lithium is a scarce element and the available resources are definitely not matching the rapidly growing demand for energy storage. Therefore, sodium- and potassium-ion batteries (SIBs and PIBs) are now considered as promising scalable metal-ion battery technologies. In that context, organic redox-active materials are particularly important since they can operate efficiently with multiple mobile ions, while most of inorganic cathodes are constrained to only one specific ion matching the crystal lattice.

In this talk, we will highlight our recent results on the design of organic and metal-organic cathode and anode materials for potassium batteries. In particular, we will present ultrafast potassium-ion batteries delivering specific capacities of 169 mA h g−1 at an impressive current density of 10 A g−1 (charging/discharging in ca. one minute) and 245 mA h g−1A at a lower current density of 50 mA g−1. Specific energy of ~550-600 W h kg-1 is reached for the best organic cathodes in potassium batteries. The polymer-based devices also demonstrated record-high cycling stability with no capacity decay after 4600 cycles, thus outperforming all previously reported non-aqueous K-ion batteries.

The obtained results suggest that organic electrode materials, while being at the infancy of their development, start to show commercially interesting performances thus paving a way to implementation of a new generation of post-lithium metal-ion batteries.

Key Words: Potassium-Ion Batteries, Energy Storage

Abstract ID: 959

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Solar Cells

Keywords: dyes sensors, energy storage, electrochromism, photochemistry, molecular electronics, charge transport

Developing Multifunctional, High Performance Thiazolothiazole Materials for Electronic and Optical Applications

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Thiazolothiazole (TTz) materials are promising molecular platforms for a variety of electronic and optical applications. We have developed TTz dye systems that can serve as an electrochromic material,(1) as a dye for biosensing applications,(2) and as a stable material for molecular electronics and energy storage. Extended TTz viologen structures demonstrate both reversible electrochromic behavior and high fluorescence quantum efficiency that is deactivated with electrochemical reduction. Water-soluble, chromogenic TTz derivatives show excellent reversibility and stable cycling in a simple aqueous, polyvinyl alcohol/borax gel electrolyte electrochromic device. They produce voltage-dependent purple or blue coloration and efficient electrofluorochromism. We have also developed environmentally sensitive asymmetric TTz derivatives can serve as molecular probes for cell imaging and cell membrane voltage sensing. These asymmetric TTz derivatives exhibit strong solvatofluorochromism with fluorescence quantum yields > 0.9. In vitro cell studies indicate good cell membrane localization, insignificant cytotoxicity, promising voltage sensitivities, and photostability that is 4 times higher than comparable dyes. Lastly, solution-processable TTz compounds can be used as charge transport layers in a variety of molecular electronic devices (OLEDs and OPVs) and as energy storage materials. Their ease of synthesis and purification, remarkable photophysical properties, and chemically sensitive TTz bridge make these materials attractive for multi-functional optoelectronic, electron transfer, electrochromic, and other photochemical / energy storage applications.

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Abstract ID: 960

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster/Oral Presentation

Topics: Electrochemical properties of graphene, Mxenes and other two-dimensional materials

Keywords: Electrochemistry, Overpotential, Hydrogen Evolution, electrocatalyst, Crystal Phase

Investigation on Electrochemical Hydrogen Evolution using different crystal phases of TaS2

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Hydrogen has recently been found as the best energy carrier, due to several advantages compared to fossil fuels. Although hydrogen evolution is a relative mature technology, the current production technologies have not met the requirements, e.g., conventional evolution systems have not offered an environmental-safe or energy- and/or cost-effective one. Here, we report an electrocatalyst for evolution of hydrogen which is comparable to the performance of global-standard electrode of Platinum. Electrochemical measurements demonstrates that electrochemical hydrogen evolution at the surface of exfoliated rhombohedral Tantalum disulfide nanosheets, immobilized on surface of glassy carbon electrode using Nafion solution as a binder, is occurred at the significant low overpotential of 0.13 V (Vs. RHE) at 10 mA/cm2. However, characterization of the trigonal crystal phase system shows a deteriorated performance toward hydrogen evolution, overpotential of 0.9 V at 10 mA/cm2. Investigation of the Tafel plot showed that the slopes for both systems are roughly the same, showing that the kinetically rate of electrochemical reaction and overpotential is comparable for the different crystal phases. Overall, it shows that the structure, which provides the different architecture and configuration of the systems, plays a key role for evolution. It translates that the confinement of sulfur atoms cannot enhance the reduction rate. On the contrary, having the sulfur at the crystal-unit boarder (rhombohedral structure) can increase the efficiency for hydrogen evolution. Higher performance also may be ascribed to the improved diffusion rate of protons toward lattice through exposure of sulfuric sites. It also suggests that hot reaction sites are located on or close to the sulfur atoms. Clearly, electron perturbation arises from heteroatom (sulfur) should also be taken into account. Moreover, calculation of active sites in both systems reveals that the number of active sites in the rhombohedral sample is higher than that of triangle one. It clearly shows that activated basal and edge sites has been formed in the rhombohedral structure.

Abstract ID: 961
Symposium 4: Functional Composite Materials (FCM)
Poster Presentation
Topics: Nanocomposites
Keywords: Graphene, Thermal management, Capillary hydrodynamics, Evaporation rate

Combined method of thermal stabilization of electronic and energy devices based on graphene hybrid nanostructures with nontrivial capillary hydrodynamics and efficient evaporation

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Recently, interest in new methods of thermal stabilization of electronic devices based on multiphase evaporative hydrodynamics has greatly increased [1]. 2D materials, in particular graphene nanochannels and membranes, are of great interest [2,3]. The paper proposes and investigates a combined method of thermal stabilization of electronic and energy devices, which is based on graphene hybrid structures as functional materials. The method is based on nontrivial capillary hydrodynamics of the flow of working fluids, including water, through nanopores and nanochannels and effective evaporation from interfacial surfaces. High flow rates of liquids, the influence of the liquid-vapor interface, as well as the features of graphene structures (regular or random) make it possible to effectively cool the surfaces and, in part, the internal regions of devices using evaporative cooling. Models of flows in nanochannels, heat and mass transfer during evaporation, and integral models for calculating thermal management are considered. Preliminary experimental results of studying heating, vapor generation, and cooling of graphene surface nanostructures are presented. New experimental data have been obtained on the effect of the size of nanopores and nanochannels on the evaporation rate, as well as the geometric structure, as well as the addition of boron nitride and aluminum nitride nanoparticles on the evaporation rate and surface cooling characteristics. By the example of the evaporation of droplets of working fluids in a wide temperature range on various substrates, including metal mesh and graphene nanoflakes, the efficiency of the removal of high heat fluxes from heated surfaces with Joule dissipation is shown. The results of this work actually continue our earlier studies [4]. It is shown that this method of thermal stabilization is very effective, has high parameters of heat and mass transfer, and allows large heat fluxes to be removed.

Abstract ID: 962

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Solar Cells

Keywords: Perovskite, Phase Segregation, Solar Cells

The origin of the light-induced phase segregation in mixed halide perovskites

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Tunability of optoelectronic properties of lead halide perovskites achieved through halide mixing can potentially enable their multiple applications e.g. in tandem solar cells and light-emitting diodes. However, mixed halide perovskites are unstable under illumination due to their segregation into Br-rich and I-rich phases, which negatively affects the performance characteristics and operational stability of devices. Research efforts over the past years provided a substantial understanding of the factors influencing light-induced halide phase segregation. While several mechanisms were proposed, none of them could account for all available experimental data; and hence the origin of the effect is still under active debate. Herein, we thoroughly investigated the photodegradation of CsPbI2Br and Cs1.2PbI2Br1.2 using a set of complementary techniques. In-situ atomic force microscopy provided a spectacular visualization of the real-time halide phase segregation dynamics demonstrating that iodoplumbate is selectively expelled from the mixed halide perovskite grains and nucleates as a separate I-rich phase at the grain boundaries. We propose a mechanism based on the reversible Pb2+/Pb0 and I-/I3- redox (photo)chemistry, which explains our experimental findings and other previously reported results. Furthermore, it sheds new insights on the underlying mechanisms of multiple phenomena related to light- or electric field-induced degradation of various lead halide perovskites. More details can be found in our recently published paper [1].

Key Words: Perovskite, Phase Segregation, Solar Cells

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Abstract ID: 963

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Industrial applications of composite materials

Keywords: rare earth recovery, urban mining, selective adsorption

Functional Pickering Emulsion extractant based on Cyanex 923-chitosan-polyethylene glycol for selective extraction of Yttrium from fluorescent lamp wastes

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A novel pickering emulsion (PE) addressed to encapsulate a selective molecule for rare earthextraction (Cyanex 923) into a biopolymer (chitosan) and a non-ionic surfactant (polyethyelene glicol 4000, PEG) has been obtained. This PE was applied as extractant emulsion for recovering Yttrium (Y) from a liquid phase containing a blend Y/Ca, which are representative elements of fluorescent lamp wastes after solid-liquid extraction. The PE was obtained by applying ultrasound cavitation in a blend of 30 mL of chitosan of 10 mg/mL, 12 mL of Cyanex 923, and 0.4 g of PEG for 2 min. and 180 W. The PE was characterized by transmission electron microscopy, confocal microscopy, dynamic light scattering, and rheological measurements. The applicability assessment towards Y extraction includes optimal dosage, pH effect, uptake capacity, selectivity, ion strength effect, and reusability tests. 69% of Y was recovered/adsorbed/removed from the Y/Ca mixture with a separation factor (β_(Y/Ca)) of 5. There is not significant impact when the pH and ion strength of the aqueous phase was varied and the material was reused up to 3 times. The PE drop size was 1 µm in average, the distribution of Cyanex 923 into the PE was homogeneous, and the viscoelastic profile of PE showed a long-term stability behavior. To the best of our knowledge, it has been demonstrated for the first time the use of a biopolymer and PEG for encapsulate Cyanex 923 and apply them in rare earth recovery from aqueous phases. This approach offers a broad applicability in the metal extraction, as it would enable to encapsulate other extractant molecules and ion liquids for a desired metal extraction application.

Abstract ID: 964

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Optical properties of metals and non-metals

Keywords: Plasmonics, Density Functional Theory, Electromagnetic Modelling, Computational Materials

Computational Design and Optimization of Future Plasmonic Materials and Nanostructures

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Working with plasmonic and electronic materials involves many scientific steps, including, aside from the laboratory-level experiments, the numerical creation, their comparison, and the device fabrication. Besides these challenging steps, the design of new plasmonic materials with unique physical and chemical characteristics, and outstanding optical properties, which are traditional realms of gold and silver, merits an important place. Optimizing the material properties to improve their functionality and performance in plasmonic applications is a subsequent challenge to be tackled, also through iterative feedback from the experiments. This presentation will demonstrate an overview of recent advances in the computational design of potential future plasmonic materials, such as translational metals, transparent conducting oxides, or plasmonically active semiconductor allotropes, and their application in plasmonic structures, concepts, and devices. The extraction of complex dispersion characteristics from density functional theory (DFT) calculations allows the integration into subsequent electromagnetic modeling steps. We specifically demonstrate the search for new alternative plasmonic materials by manipulating the characteristic response of material candidates such as Al/Ga doped Zinc Oxide (A/GZO), ZrN, TiN and Silicon allotropes. We first perform a series of DFT calculations, including the structural relaxation of plasmonic material candidates, to find the crystal structure with minimum energy, for different exchange-correlation functionals such as GGA, LDA. Secondly, we analyse the simulated material's electronic and optical properties to illustrate potential metallic behaviour, via the electronic density of states (DOS) and subsequently extracted optical dispersion parameters, such as complex refractive index data, Drude-Lorentz parameters, and complex dielectric permittivity. These dispersion data can finally be fed into any electromagnetic simulation tool appropriate to any desired optical system, to investigate its efficiency for suitability in plasmonic applications. Our method comprises the possibility for verification with experimental data on each level. It further admits optimizing digitally the molecular structure, paving the way to predict the proposed compounds' plasmonic functionality, overcoming the persistent hurdles introduced by pure experimental works. We will further introduce the recently developed "Photonic Materials Cloud," a cloud-based platform to support streamline the experimental, numerical, research, and education-based work on plasmonic materials. It allows for creating and comparing various material data via various methods and applying them to standard photonic or plasmonic applications, such as nanoparticle scattering and layered thin-film responses. The export of publication-ready graphics and column-based data facilitates its easy integration into a photonic materials science research line.

Abstract ID: 965

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Nanoparticles, Nanowires, and 3D Structures

Keywords: III-V semiconductors, Surfaces, Interfaces, Nanostructures, STM

Atomic-scale surface characterization of (opto)electronic III-V semiconductor nanowire devices

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Semiconductor nanowires are promising candidates for next generation (opto)electronic and photovoltaic devices, such as solar cells made of InP pin-junction nanowires [1] or tunnel FETs based on InAs-GaSb axial nanowire heterostructures [2]. III-V semiconductor nanowires with superior charge carrier mobility and direct bandgap can be epitaxially grown on silicon substrates without interfacial defects, enabling quantum-size effects with a large flexibility in combining different materials. Due to the small size and high aspect ratio of nanowires, their properties are to a significant extend determined by surface effects. Therefore, atomic-scale surface and interface characterization is crucial for understanding and improving the performance of nanowire-based devices.

Here, I will present our toolbox for complementary and atomic-scale surface characterization of III-V semiconductor nanowires, based on scanning tunneling microscopy and spectroscopy (STM/S), atomic force microscopy, and synchrotron X-ray imaging and spectroscopy methods. We map heterostructures between different doping levels [3], materials [4,5], or different crystal phase [6-8], where we correlate the surface structure and local electronic properties across the interfaces of axial nanowire heterostructures. Recent efforts include in-operando and in-situ studies, where we investigate nanowires during device performance [3,4] or while their surface becomes modified [8].

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Abstract ID: 966

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Multifunctional composites

Keywords: α-Ag2-2xCuxWO4 solid solutions; Morphology; Biocide activity; DFT study

Biocide activity of α-Ag2-2xCuxWO4 ($0 \leq x \leq 0.16$) solid solution: Theory meets experiments

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In this work, α-Ag2-2xCuxWO4 ($0 \leq x \leq 0.16$) solid solution with enhanced antibacterial (against methicillin-resistant Staphylococcus aureus) and antifungal (against Candida albicans) activities are reported. Different techniques (X-ray diffraction with Rietveld refinements, and spectroscopies of attenuated total reflectance-Fourier transform infrared, Micro-Raman, and inductively coupled plasma-atomic emission, ultraviolet-visible diffuse reflectance, X-ray photoelectron, field emission-scanning electron microscopy, and photoluminescence emissions) have been employed to characterize the as-synthetized samples. To find a correlation between morphology and biocide activity, the experimental results are sustained by first-principles calculations, at the density functional theory level, to decipher the geometry and electronic properties of the exposed surfaces. Based on the analysis of the undercoordinated Ag and Cu clusters at the (010) and (101) surfaces, we share some speculative insights into possible action mechanism to explain the biocide activity of this material.

Abstract ID: 967

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Transparent Conductors

Keywords: AZO, rare-earth, terbium, luminescence, energy transfer

Terbium doping and luminescent activation effects on the optical and luminescent properties of aluminum zinc oxide thin films

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Rare-earth doped wide bandgap (WBG) semiconductors have attracted great attention as efficient luminescent materials for optoelectronic applications, such as photon downshift, down- and up- conversion systems, a new generation of low voltage light-emitting devices, non-contact luminescent temperature sensors and photonic structures. However, the luminescence activation of rare-earth ions is yet to be successfully achieved in transparent conductive oxide (TCO) films, such as indium tin oxide (ITO) or aluminum zinc oxide (AZO) which also have a WBG and often form part of those structures and devices. Such optically active TCOs would therefore be advantageous for these applications. Our work focuses on the production and characterization of terbium (Tb) doped AZO thin films, keeping a high optical transmittance in the visible region and exhibiting Tb3+ characteristic luminescence. The effect of Tb doping on the optical and luminescent properties was investigated for different post-deposition annealing conditions. Films were produced on silicon and fused silica substrates by radiofrequency magnetron co-sputtering employing high purity AZO and Tb targets. Samples were annealed post-deposition between 200°C - 1000°C in air or argon ambient. Optical transmittance, spectroscopic ellipsometry, photoluminescence (PL), cathodoluminescence (CL) and energy dispersive X-ray spectroscopy experiments were made after each annealing step. As grown and annealed samples revealed characteristic Tb3+ emission. Absorption coefficient, band gap and Urbach energies were estimated using computational methods and models developed in our group. PL and CL results suggest an indirect excitation mechanism of activated Tb ions. To further assess this possible mechanism, temperature dependent PL experiments, ranging from -190 °C to 300 °C, were carried out on representative samples. It is proposed that excitation energy is transferred from bound excitons to activated Tb3+ clusters. This is tentatively modeled using a spherical potential well, as well as a tight-binding one-band approximation approach for a short-range charge trapping process and subsequent formation of bound excitons to rare earth ions clusters.

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Abstract ID: 968
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Bio-composites
Keywords: PVC-SiO2-Ag composite, biocide material.

PVC-SiO2-Ag composite as powerful biocide material

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The ongoing COVID-19 pandemic has pushed scientists and technologists to find novel strategies to develop new materials and structures able to meet challenging goals such prevention, transmission, and proliferation of microorganisms. In this report, the fabrication of polyvinyl chloride (PVC)-SiO2-Ag composite is presented. We evaluate the activity of this materials applied to eliminate bacteria (Staphylococcus aureus, Escherichia coli), and fungus (Penicillium funiculosum), and SARS-CoV-2, by contact. This research and innovation front can be considered as a breakthrough for the design of biocide materials. Future directions for this exciting and highly significant field of research can open the door to the development of new technologies for the fabrication of packaging films to protect consumer products (such as fruits, vegetables, food).

Abstract ID: 969

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Anodes and cathodes Materials

Keywords: non-graphitizing carbons, structure, anode materials, lithium-ion batteries

Developing of Non-graphitizing Carbons as Alternative Materials for Anodes in Li-Ion Batteries

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Carbon anode materials are still under intensive investigation to improve their specific capacity and cycle life in Li-ion batteries [1]. Some non-graphitizing carbon materials prepared by pyrolysis of hydrogen-rich precursors have demonstrated a capacity of more than 1000 mAhg-1, but they have a high irreversible capacity in the first cycle and short cycle life [2]. Therefore, attempts have been made to modify their structure towards better electrochemical properties. We developed glassy carbon and sucrose-based carbon materials modified with various non-carbon additives, which have a catalytic effect on the structural transformation during the graphitization process. The additives are completely removed from the carbon matrix during the heat-treatment at 3000°C. The obtained structures have atypical fiber-like morphology, high degree of graphitization, low surface area and high density, which make them interesting candidates for use as anode materials. By tailoring the type and concentration of the additives, it is possible to optimize the carbon matrix to deliver the structure with the desired properties. They will be compared with the properties of carbons based on graphitizing coke, commonly used as anode material.

Abstract ID: 970
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Industrial applications of composite materials
Keywords: Boron Nitride, Reactive Ion Etching, Thin Film Pressure Sensor

Self-adjusting boron nitride mask for Reactive-Ion Etching

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In this paper a simple approach is demonstrated for spatially selective etching of a silicon nitride layer by Reactive Ion Etching (RIE) by using a reusable shadow mask as a separate solid component part. Two ceramics were compared as mask materials: aluminum oxide and boron nitride. After the usage of an aluminum oxide mask several times, the deposition of small aluminum fluoride particles is observed. In contrast, using a boron nitride mask, a RIE process without any residuals on the surface can be accomplished. Furthermore, cutting a shadow mask out of bulk material, containing a three dimensional structure, is feasible.

Abstract ID: 971

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Superconductivity and Superfluidity

Keywords: BiS2-based superconductors, Layered materials, Pb-substitution, Resistivity, DC susceptibility

Pb–substitution in Eu3Bi2S4F4: A superconductor to insulator transition

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Discovery of superconductivity in BiS2–based compounds suggest the possibility of emergence of new high temperature superconductors from this family. They possess similar layered structure as in cuprates and iron–based pnictides. After discovery of superconductivity in Bi4O4S3 (Tc = 4.5 K) various BiS2–based systems were formed by changing the composition of block and conduction layer in the layered structure. LnO1-xFxBiS2 (Ln = La, Ce, Pr, Nd, Sm and Yb), Ln1-xMxOBiS2, Sr1-xLnxFBiS2 (Ln = La, Ce, Pr, Nd and Sm), EuFBiS2 and Eu3Bi2S4F4 superconductors have been known. In an attempt to introduce holes in the system Sr–doping at La–sites in LaOBiS2 was tried. But hole–doping is not found to induce superconductivity in LaOBiS2. The structural and mixed valence properties of the Eu–based EuFBiS2 and Eu3Bi2S4F4 superconductors have been discussed in literature. Effect of isovalent Se–substitution at S–sites leads to remarkable increase in Tc in both systems.

We have investigated effect of doping lead at bismuth site in Eu3Bi2S4F4 superconductor (Tc ~ 1.5 K). Lattice parameters and hence unit cell volume decreases gradually on increasing Pb–content in Eu3Bi2-xPbxS4F4 (x = 0.25, 0.5, 0.75 and 1). The systematic decrease in cell volume suggests successful incorporation of Pb in the lattice. Remarkably, Pb (x = 0.25) destroys superconductivity and a highly insulating state is obtained. The susceptibility measurement shows that for x = 0.25 sample the value of magnetic moment is smaller as compared to the Pb–free compound, but in higher Pb–content the variation of magnetic moment is (±) 0.2–0.5μB. The variation in magnetic moment in Pb– substituted samples suggest mixed valence state associated with the Eu–ions.

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Abstract ID: 972

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: Methanol synthesis, Cu nanoparticles, Gallium Oxide, atomic and molecular simulation, DFT

DFT Investigation of CO2 Hydrogenation to Methanol over dispersed Cu particles on Ga2O3 Surface

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Methanol is an important feedstock in chemical industries and can be alternative to fossil fuels. Methanol synthesis from CO2 hydrogenation has been of great attention to reduce the CO2emissions and recycle carbon [1]. Methanol formation by CO2 hydrogenation occurs via the following reaction

〖CO〗_2+3H_2→〖CH〗_3 OH+H_2 ΔH_r=-52 kJ/mol

over the well-known commercial catalyst Cu-ZnO supported by Al2O3 at50–100 bar and 200–300 °C, and the reverse water-gas-shift (RWGS) reaction also accompanies to this reaction

〖CO〗_2+H_2→CO+H_2 O ΔH_r=42 kJ/mol

and CO is produced as an unwanted by product.The rate of methanol formation in terms of these two reactions are thermodynamically and kinetically limited. Therefore, in order to increase the activity and selectivity to methanol,some other metal promotions to copper based catalyst have been still under investigation. It was observed that Ga promotion enhances the activity and selectivity [2].We have been carried out a DFT study to investigate the effect of the interaction of copper nanoparticles and Ga2O3 surface on the CO2 hydrogenation reaction for methanol production. To that end, 6-layer-(2x3)Ga2O3(001) surface was prepared and 4-atom Cu cluster was adsorbed on this surface.

Our motivation is that, the copper nano particlesis able to promote the hydrogen dissociation[3] and Ga2O3 activates the CO2 hydrogenation [4] for methanol synthesis.

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Abstract ID: 973
Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)
Invited Talk
Topics: Nanoparticles, Nanowires, and 3D Structures
Keywords: upconverting nanoparticles, near infrared imaging, nonlinear optics, lanthanides

Photon avalanching nanoparticles for NIR imaging at 70 nm resolution

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Photon avalanching nanoparticles for NIR imaging at 70 nm resolution

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Avalanches are steeply nonlinear events in which outsized responses arise from a series of minute inputs. With light, photon avalanching (PA) enables technologies such as optical phase-conjugate imaging, IR quantum counting, and efficient upconverted lasing. However, PA has been observed only in bulk materials and aggregates, often at cryogenic temperatures, preventing its application to bioimaging. We have recently reported the realization of PA at room temperature in sub-30 nm Tm3+-doped upconverting nanocrystals and demonstrate their use in high-resolution imaging at wavelengths that fall within NIR spectral windows of maximal biological transparency.1 Avalanching nanoparticles (ANPs) can be pumped by either continuous-wave or pulsed lasers and exhibit all of the defining features of PA: clear excitation power thresholds, exceptionally long rise time at threshold, and a dominant excited-state absorption that is >10,000 times larger than ground-state absorption. Beyond the avalanching threshold, ANP emission scales with up to the 31st power of pump intensity, an extreme nonlinearity caused by the induced positive optical feedback within each nanocrystal. This enables the experimental realization of photon-avalanche single-beam superresolution imaging (PASSI), achieving sub-70 nm spatial resolution using only simple scanning confocal microscopy and before any computational data analysis. NaYF4 ANPs with 8-20% Tm3+content can be excited at either 1064 or 1450 nm, with avalanching emission at 800 nm. Pairing the steep nonlinearity of ANPs with existing superresolution techniques and computational methods allows for imaging with higher resolution and at ca. 100-fold lower excitation intensities than is possible with other probes.

1. Lee, C. et al. Giant nonlinear optical responses from photon-avalanching nanoparticles. Nature 589 (2021), 230–235.

Abstract ID: 974

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Sensors and MEMS: Materials and Devices

Keywords: SERS, bacteria, sensor, virus, plasmonics, nanoparticle

Surface enhanced Raman spectroscopy for bacterial and viral detection

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Clean air and clean water are critical requirements for environmental sustainability. To assure the quality of these matrices, we currently rely upon a broad range of monitoring techniques - many of which are outdated, unreliable, or excessively expensive. Recent advances in both nanotechnology and biotechnology, however, are poised to provide novel and previously unattainable alternatives that have the potential to be more sensitive as well as more cost-effective than many existing methods. In this presentation, we will present work conducted to develop gold enabled plasmonic platforms that facilitate detection of inorganic, organic, biologic, and nanoparticulate contaminants. As will be shown, Raman spectroscopy and surface enhanced Raman spectroscopy (SERS) can both be used to detect and quantify environmental contaminants in a range of different media.

Abstract ID: 975

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Computational modeling and simulation for energy storage and conversion devices

Keywords: Lithium-ion Battery, Detailed Modeling, Multi-physics

Detailed Multiphysics Modeling of a 18650 Cylindrical Lithium-ion Battery

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In this fast-growing electrification era, need for higher energy density and safer batteries to be used in various applications sparks researchers' interests from different fields of study to analyze this multi-physics and multi-scale phenomenon. The layered structure of the lithium-ion batteries includes combination of various components which have different mechanical, electrical and thermal properties. The coupled effects of these physics has made battery modeling a complex problem. Hence, a cost-efficient model to precisely predict the behavior of batteries is in high demand by all the battery related industries. Several publications have investigated the mechanical behavior of batteries in different loading scenarios but a detailed modeling of a battery validated in coupled loading scenarios hasn't been completed. In this study, first a conditioned battery cell was dissected, and samples were prepared from the jellyroll layers. A variety of testing was done on the samples to measure mechanical, electrical and thermal properties of the layers. The structure of the cell components and in-situ jellyroll configurations were extracted using CT-scan of the battery. A model for the cell was developed in ABAQUS Explicit to simulate a combined mechanical electrical loading scenario. The detailed model was validated under combined mechanical/electrical/thermal loading. This comprehensive detailed modeling and the material calibration provide in this study, create a tool for various battery related industries to optimize properties of their products by using battery cell modeling and investigate effects of various component changes or safety features on a fully coupled detailed model. This tool will reduce the timing and costs of the design and development steps to manufacture a safe and high energy/power density product.

Abstract ID: 976

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Poster/Oral Presentation

Topics: Sensors and MEMS: Materials and Devices

Keywords: anic scintillator, additive manufacturing, stereolithography, radiation detection

3D Printing a Plastic Scintillator for Radiation Detection

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The objective of this work was to create an unobtrusive, discreet radiation sensor. In this paper we describe the additive manufacturing process used to fabricate an organic scintillator for use in a radiation detector. An off the shelf stereolithography printer was used with commodity clear resin which was doped with different scintillant powders in varying amounts to improve the resulting scintillation function of the resulting resin formulation. The concentration of the dopant, the method of mixing, and the overall printing process was investigated to produce an additively manufactured scintillator which was then coupled with a standard photomultiplier tube to detect radiation. The radiation detector was tested with gamma and neutron radiation sources over varying exposure periods. The detector with a 3D printed scintillator was able to clearly distinguish the radiation sources from background with fluorescent response relative to the strength and energy of the source and with sensitivity comparable to a commercial organic or plastic scintillator. The scintillation behavior when exposed to ionizing radiation is analogous to the way the material fluoresces when exposed to UV light (e.g. a black light), samples of 3D printed plastic scintillators are shown in Figure 1. Future work will include customization of the geometry, coupling to other light sensors, and expansion to other printing methods, and evaluation of the ability to further discriminate ionizing radiation sources to create an effective and discreet detector.

Abstract ID: 977

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Topological Insulators, 2D Materials, and Voltage Controlled Magnetism

Keywords: Graphene, 2D-layered vdW ferromagnetic materials, Topological insulator, Room temperature, Spin orbit torque

Room-temperature ferromagnetism in 2D vdW Fe3GeTe2 and its potential application

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Since the discovery of single-layer graphene in 2004, two-dimensional (2D) van der Waals (vdW) materials represented by it have demonstrated excellent electrical, magnetic, mechanical and optical physical properties under the structure of one or several layers of atomic thickness. Based on these superior properties, 2D-layered vdW ferromagnetic materials have become the basis for constructing low-dimensional spintronics devices, in which Fe3GeTe2 (FGT), Cr2Ge2Te6 and CrI3 as the main representative materials exhibit strong perpendicular magnetic anisotropy and other important characteristics in single layer. However, the Curie temperature (Tc) of above materials has not reached room temperature yet, which has greatly hinderer the subsequent development for device application. Therefore, recently researchers have been committed to explore 2D vdW ferromagnetic materials for room-temperature Tc in both theory and experiment. Here, we report that the interfacial engineering effect could effectively increase the Tc of the 2D vdW ferromagnetic material FGT from 230 K to 400 K, through heteroepitaxy with topological insulator of Bi2Te3. A theoretical calculation was further carried out to describe the magnetic properties by using first-principles calculations and the self-consistent Hubbard U approach (DFT+Uscf) together with the Monte Carlo (MC) simulations. After combination with Bi2Te3, the intralayer interactions in FGT was calculated to dramatically increase compared to that in pure FGT, well explaining the Tc enhancement. Furthermore, we realize the high-efficiency SOT switching of Bi2Te3(8)|FGT(4) at room temperature with a write current density of 2.2×106 A/cm2 through electrical transports. The experimental analysis of harmonic voltage measurements displays that the topological surface state of Bi2Te3 at room temperature has achieved the magnetization switching of FGT as the main contribution. In particular, the thermal effect in the heterostructure can be reduced by varying the thickness of FGT, which originates from the large anomalous Nernst effect of FGT. Moreover, we report the oxidation process of FGT films exposed to the atmospheric air, which was studied by X-ray photoelectron spectroscopy measurements. The conclusion provides information for the subsequent growth and protection of FGT films, which facilitates the in-depth study of other properties. Our results may open up a new door to benefit the magnetic order in the 2D limit and realize spintronic devices based on 2D-layered vdW ferromagnetic materials with room temperature performances towards industrialization.

Abstract ID: 978
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Smart Composites
Keywords: energy method, modified strength of materials method, piezoelectric composites, smart composites, composites, FRC

Micromechanics of piezoelectric fiber reinforced composites using modified strength of materials and energy approaches

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The effect of fiber cross-section on effective elastic and piezoelectric coefficients of piezoelectric fiber reinforced composites (PFRC) is investigated through two micromechanical methods viz. modified strength of materials (MSM) approach and energy approach. Results are verified with that of strength of materials (SM) approach available in the literature. A constant electric field is considered in the direction transverse to the fiber direction and is assumed to be same both in the fiber and matrix phases. It is observed that MSM and strength of materials (SM) approach predictions for the effective piezoelectric coefficient of the PFRC assessing the actuating capability in the fiber direction are in excellent agreement and also when the fiber volume fraction exceeds a critical value, this effective piezoelectric coefficient becomes significantly larger than the corresponding coefficient of the piezoelectric material of the fiber as investigated by both SM and MSM approaches. However, results of energy approach differ from both MSM and SM results and effective piezoelectric constant never exceeds to that of fiber as obtained by energy approach. It has been found for the piezoelectric fibers, cross-section of fiber has insignificant effect on the effective properties as predicted by MSM and energy approaches.

Abstract ID: 979

Symposium 4: Functional Composite Materials (FCM)

Poster Presentation

Topics: Experimental methods for Composite materials

Keywords: Bisphenol, Paraben, Electropolymerization, PEDOT, lignosulfonate

Electropolymerized sorbents for determination of potential endocrine disruptors in environmental samples

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Several conducting polymers were tested as sorbent materials for the extraction of potential endocrine disruptive compounds from aqueous solutions. Six bisphenols and five parabens were the environmental pollutants selected for this experiment because of their wide range of applications in consumer products [1,2] and presence in the various environmental matrices [3] that can lead to endangering the ecosystem.

The electropolymerized sorbents tested in the study included: polypyrrole, poly(3,4-ethylenedioxythiophene) (PEDOT), and its composite with lignosulfonate (PEDOT/LS). Both sorbents were used in solid-phase microextraction and allowed for the extraction of bisphenols and parabens from water samples before their chromatographic determination in the LC-MS/MS system. Bisphenols were determined using a procedure with PEDOT/LS sorbent while parabens with the PEDOT sorbent.

Various parameters influencing both methods were optimized including the type of sorbent, time of electropolymerization, preconditioning, extraction time, desorption (time and solvent used), and pH of the aqueous sample. Under optimal conditions the proposed methods allowed to achieve good precision (n = 5) ranging between 6.0 and 12.1% for bisphenols and 5.7 and 11.8% for parabens, and recovery levels of 73.8 - 102.8% and 70.1 - 98.0%, respectively. The limits of detection for bisphenols ranged between 0.03 and 0.17 μg L-1, for parabens between 0.004 and 0.28 μg L-1. The proposed methods were successfully applied for the determination of bisphenols and parabens in aqueous environmental samples giving great selectivity and sensitivity.

Abstract ID: 980

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Artificial photosynthesis

Keywords: 2D graphenic semiconductors, Photocatalysis, CO2 reduction, water splitting

Biomimetic Fe-decorated P-doped carbon nitride catalyst for glycerol assisted photo-reforming of furfural to furfuryl alcohol.

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The staggering CO2 concentration and inflated energy demand have brought up the urgency to adopt carbon-neutral technologies to minimize carbon footprints. Lignocellulosic biomass is the largest available chemical feedstock that upon thermal pyrolysis and fractionation produces C5 and C6 furanic such as furfural, hydroxy-methyl-furfural (HMF). These platform chemicals can be transformed into value-added chemicals using catalytic hydrogenation. Conventional hydrogenation approaches are energy-intensive requiring high operating temperature, pressurized hydrogen and noble metal-based catalysts which suffer from deactivation under such conditions. Sustainable synthesis of green chemical conjugates from abundant biomass using solar light and semiconductor catalysts can fulfill our energy/chemical demands while leveling off the CO2 concentrations. Several semiconductor photocatalysts have been developed in past decades to promote various photo-redox reactions including CO2 reduction, water splitting however afforded efficiency is far from the realization value due to limited absorption, fast carrier recombination, poor visible absorption and sluggish water oxidation reaction demanding high oxidation potential. The photocatalytic reaction kinetics can be accelerated using biomass derivatives with a relatively low oxidation potential which upon oxidation at the valence band can produce valuable chemicals while supplying required hydrogen for the reduction of another platform chemicals at the conduction band. 2D graphenic carbon nitride-based semiconductors constituted of sp2 hybridized 2D network of N-bridged C6N7 (heptazine) units have emerged as potential photocatalytic materials due to their excellent chemical, physical and optical properties such as tuned bandgap, thermal and chemical stability, excellent charge carrier mobility and multitudinous active sites. The change in the chemical constitution of carbon nitride via P doping in the C6N7 network has been found to increase the visible absorption profile in the visible regime. Unfortunately, existing protocols utilize expensive ionic liquids such as BMiMPF6 reaching a maximum 0.5% P dopant concentration while the observed reduction in bandgap remains due to C and F co-doping. Herein we have achieved a benchmark 3.2 % P doping in carbon nitride framework using cheap precursor while avoiding co-dopants under a closed system which displayed a significant reduction in bandgap reaching 1.4 eV. When decorated with iron in a highly dispersed state, the developed photocatalysts can couple two redox reactions 1) oxidation of glycerol to glyceraldehyde at EVB and 2) reduction of furfural to furfuryl alcohol at ECB from generated protons from the oxidation of glycerol.

Abstract ID: 981
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Processing and manufacturing technologies
Keywords: Microfluidics, Engraving, Plasma Treatment, Solvent, Bonding

Polymer-polymer Bonding for Enhanced Functional Microfluidic Chips Fabrication

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Polymer-polymer Bonding for Enhanced Functional Microfluidic Chips Fabrication

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Low-cost and easy fabrication of polymer-based microfluidic devices are of great potential for many biomedical and environmental applications1. Different microchannel designs are employed for various fluid mixing/separating techniques, such as valving, pumping, centrifugation, and filtration. Polymethyl methacrylate (PMMA) is highly attractive for fabricating disposable microfluidic devices because of its optical clarity, chemical compatibility, reasonable robustness, and ease of fabrication. Pressure sensitive adhesive (PSA) is used for binding microchip parts and provides a good sealing2. However, PSA layers are difficult to align precisely. They may cause clogging of microchannels, reducing chip transparency and affect the functionality of chips that are dimensionally sensitive. Direct polymer-polymer bonding at the chips-interface, if attained appropriately, leads to perfectly bonded, transparent, and easily assembled microchips3. In this study, microfluidic chips with different geometries of microchannel are fabricated. The polymer-bonding between the chip-parts is achieved a by well-defined procedure, Figure 1. The functionalities of all microfluidic chips are tested and characterized. An optimized method of microfluidic chips fabrication is reported.

Key Words: Microfluidics, Engraving, Plasma Treatment, Solvent, Bonding

Figure 1: Schematic of microfluidic chip fabrication/bonding procedure.

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Abstract ID: 982

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Photonic devices and applications

Keywords: polymer, fluorescence, solid-state emission, multicolor, through-space charge transfer

Color Tuning of Single-Fluorophore Emission via Polymerization-Mediated Charge Transfer

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Organic light-emitting materials have attracted much attention due to their great potential for various applications, such as organic light-emitting diodes, fluorescent sensors, bioimaging, and disease diagnostic. For practical use, it is essential to design the light-emitting materials with tunable multicolor emission on demand, especially for that in the solid-state. The current systems rely on the sophisticated synthesis of varied organic/polymeric fluorophores with different emission maxima, which often requires complex synthesis approaches with multiple steps and high costs. Recently, single organic fluorophore molecules were found to show multicolor or even white emission by changing the aggregate structures. This is achieved by varying the molecular packing through chemical modification, thermal treatment, or solvent exchange. However, this strategy requires precise engineering of the polymorphic state of the fluorophore molecules, which can be influenced by the environment during the manufacturing process. Therefore, robust multicolor emissive systems with simple chemical composition are still lacking. Here, a new strategy for the preparation of simple and tunable multicolor organic emissive systems was developed via aggregation-dependent single fluorophore molecule. A series of fluorescent polymers with varied molecular weight were synthesized by atom transfer radical polymerization. Their fluorescence properties were investigated in aggregated state including both in bulk and nanoparticles. The polymers exhibited strong aggregation-induced emission (AIE) and polymer chain length-dependent fluorescence color, via simple macromolecular engineering. This strategy enables the efficient modulation of the molecular fluorescence in solid state by simply varying the molecular weight of the fluorophore-polymer conjugates via controlled radical polymerization.

Abstract ID: 983

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Bio and Chemical Magnetism and Magnetic Fluids

Keywords: Micromagnetometry, spin crossover, molecular magnetism, magnetic biosensor

Perspectives of ultrasensitives magnetic sensors “Sensors 3.0 : Nanoscience & Bio-physics devices”

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Promising generation of room temperature micro/nano-sensor «Sensor 3.0» based on micromagnetometry devices for indirect detection of hysteresis switching loops in addressable nanoparticle named Spin Cross-Over Materials (SCO) will be presented. An ensemble of [Fe(hptrz)3](OTs)2 nanoparticles with a volume of ca. 3×10-3 mm3 has been investigated and given rise to 100 nV detection signal. Further improvements to the device have been achieved for the enhancement of the sensitivity, reducing noise, and the implementation of a new concept based on a differential method for a more accurate detection. These advances permit the increase of the sensitivity by 4 order magnitude of the magnetization detection3 (10-14 emu) in comparison to the SQUID (10-10 emu). This optimization provide us an original microdevice, portable, flexible and easily integrated in electronics for detecting at room-temperature very few amount of nanoparticles. This original and ultrasensitive experimental developments represent significant breakthroughs within the field of molecular magnetism. For bioSensing devices, a first evidence of femtomolar detection will be discussed based on very recent achievements.

Abstract ID: 984

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Bio-composites

Keywords: Hydroxyapatite (Hap), Egg shell, composite, chitosan (CS), bone tissue engineering

Synthesis and characterization of hydroxyapatite-reinforced chitosan composite hydrogel for bone tissue regeneration

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reinforced chitosan composite hydrogel have emerged as promising biomaterials for tissue engineering applications[1]. This is a relatively new and emerging interdisciplinary field that applies the knowledge of bioengineering (the life sciences) and the clinical sciences towards solving the critical medical problems of tissue loss and organ failureThe aim of this work was to fabricate an injectable porous scaffold material hydroxyapatite (HAp)/ chitosan composite hydrogel and investigate its potent application in bone tissue engineering[2]. However, the hydroxyapatite was successfully synthesized from eggshells waste and confirmed by various chemical's techniques[3].

Hydroxyapatite was successfully synthesized using eggshell waste as a raw material. Eggshell waste and orthophosphoric acid were co-precipitated for 2 h at an ambient temperature. The pH of the solution was adjusted to 10 using ammonium hydroxide. Then, 10–30 wt% of hydroxyapatite was loaded into the chitosan film. Furthermore, the hydroxyapatite (HAp)/chitosan (CS) composite has been confirmed by scanning electron microscopy (SEM), thermogravimetric analysis (ATG), X-ray diffraction (DRX), Fourier transform infrared spectroscopy (FTIR) and the swelling behavior of the composite was observed in phosphate buffer saline solution.

Finally, the hydroxyapatite (HAp)/chitosan (CS) composite presented good excellent properties as a tissue engineering material.

Abstract ID: 987

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Shape-memory alloy

Keywords: Soft Sensor, Shape Memory Alloy Spring, Long Short-Term Memory Neural Network, Stiffness and Self-Sensing.

Self-Sensing the Stiffness of SMA spring by Soft Sensor

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Self-Sensing the Stiffness of SMA spring by Soft Sensor

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In Intelligent Robotics and bio-engineering system, it needs an active structure that can change their mechanical characteristics & transfer their action to the passive structure. The SMA spring having variable stiffness is the perfect solution for it. A deep learned Artificial Intelligence (Long Short-Term Memory) based soft sensor of the stiffness of SMA spring is developed in this work.

A deep learning approach that can cope with nonlinearity instead of trying to engineer the perfect linear sensor. The deep learned soft sensor (Long Short -Term Memory Neural Network) is developed in three stages which are far better than other existing methods. In the first stage, the 2240 instantaneous experimental data values of Force, displacement, and the voltage across Shape Memory Spring are collected by data acquisition card at various joule heating current (1.0A,1.5A, and 2.0A). These are easy to measure variables of SMA spring and from the voltage of the SMA spring, the stiffness is predicted. The voltage across the SMA spring considered as input and stiffness as an output. In the second stage, the LSTM Neural Network is defined, and Network parameters are set. These data values are preprocessed such as normalization (scaling) and divided into 70% and 30% for training and testing. Then the data is passed to LSTM which is trained using a 70% data set. In the third stage, the trained LSTM is tested for unseen 30% data and maximum error established.

The unseen data values of the voltage of the SMA spring (30%) are used to predict the stiffness and it found that accuracy is more than 97.142 %. The RMSE is used to compare the result with another method such as polynomial. The RMSE is less than 0.1572. Also, the diagonal element (1.0) indicates the perfect correlation with itself, and the off-diagonal element (0.9849) of the correlation coefficient matrix says that there is a strong statistical correlation between the predicted variable and the measured variable. So, the result found satisfactory for unseen data.

This paper proposes a deep learned soft sensor for the prediction of self-sensed variable stiffness actuation of SMA spring. The result of the LSTM based deep learned soft sensor matches the real values of stiffness. It is also compared with the polynomial method and it is far better.

Key Words: Soft Sensor, Shape Memory Alloy Spring, Long Short-Term Memory Neural Network, Stiffness, and Self-Sensing.

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Abstract ID: 988

Symposium 4: Functional Composite Materials (FCM)

Invited Talk

Topics: Design and application of composite structures

Keywords: material gradation, Elasto-plastic analysis, Cylindrical vessel, Thermal gradient, Internal pressure, DTM

Elasto-plastic analysis of cylindrical vessel with arbitrary material gradation subjected to thermo-mechanical loading via DTM

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For the first time, response of the functionally graded (FG) hollow cylinder vessel with arbitrary material gradation in radial direction subjected to thermo-mechanical loads is investigated by employing differential transformation method (DTM). The coordinate transformation and proper scale factor are applied to eliminate redundant terms in DTM, as result fast convergence with less computational efforts is observed. The elasticity modulus, thermal expansion coefficient, thermal conductivity and yield stress are assumed to be arbitrary functions of radius. The thick-walled FG reservoir is in steady-state condition and strain hardening in plastic zone is neglected by using elastic-perfectly-plastic behavior assumptions. The incompressible plastic deformation and plane-strain condition are considered to obtain radial displacement in the plastic zones. The effects of various parameters on commencement and propagation of possible plastic zones, yield pressure and yield temperature gradient are investigated. The analytical solutions for FG cylindrical container with conventional power law gradation are presented. In the case of arbitrary material gradation, the validity of the numerical procedure is proved by observing convergence and good agreement between results of DTM and results of finite element software Abaqus.

Abstract ID: 989

Symposium 4: Functional Composite Materials (FCM)

Poster/Oral Presentation

Topics: Bio-composites

Keywords: bioengineered scaffold, HAP, BTO, bone

Investigation of Bioengineering Composite Bone Scaffolds

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Barium Titanate (BTO) for its superior mechanical and piezoelectric properties and hydroxyapatite (HAP) with good bioactivity due to it naturally occurring in the human bone have been widely investigated as composites for bone tissue engineering applications. However, generally, a higher volume fraction of BTO is required, to match the mechanical and piezoelectric properties of bone. Also, there is a need for biomaterial scaffolds to follow standards for testing, only 0.3% of the publications on tissue-engineered scaffolds have referenced ASTM Standards, emphasizing the need to adhere to standards for scaffold dimensions and testing methods. In this study BTO-Hap scaffolds with Poly Vinyl Alcohol (PVA) binder, fabricated and compression tested as per the ASTM D695-15 Standard, which is the prescribed method to obtain the compressive strength in ASTM F2150-19-11, the standard guide for characterization and testing of biomaterial scaffolds used in regenerative medicine and tissue-engineered medical products. Compressive strength of 110 MPa is obtained, which is in the range for the human cortical bone with only 50% volume fraction BTO thereby preserving its bioactivity with 50% HAP. The piezoelectric coefficient, d33 has been found to be 2 Pc/N after poling, where few papers have reported a similar value with higher BTO volume fractions. The improved mechanical performance with equal amounts of BTO and Hap can be attributed to the fine and homogenous grain size and smaller pores. This has been achieved by the two-step milling process prior to and after the addition of binder, before sintering the scaffolds. This study demonstrates a robust material processing technique, which can deliver scaffolds with better electromechanical properties, tested as per ASTM Standards.

Abstract ID: 990

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: All solid-state batteries

Keywords: Solid state battery, super Capacitors, MBP, Boundary layers, Phase change

Some aspects of Energy Storage in Solid State Batteries and Capacitors

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Solid State Batteries are a choice for energy storage and retrieval in high temperature environments. Due to their ability to withstand high temperatures, elimination of spillable electrolyte and storage density, they are suitable for military,.space and industrial power application.

In this paper the mass and thermal transport mechanisms together with geometrical considerations are developed into a model amenable to analytical analysis. The effects of porosity in the solid electrolyte together with interactions with electrokinetic and diffusive parameters are varied with temperature. A set of coupled equations is obtained which is decoupled and solved for. Eigenvalies are obtained and the thermal, mass and electrokinetic boundary layers evaluated. The results are applicable to the design of more efficient and environmental friendly rechargeable power sources.

Abstract ID: 991

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Epitaxial Materials and Devices

Keywords: Quantum Materials, Oxide Heterostructures, Surface and Interface, Synchrotron X-ray Studies, Phase Retrieval

Atomic Imaging Functional Heterostructures and Interfaces by Phasing Coherent Bragg Rods for Quantum Materials

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Ubiquitous in a wide range of nature processes and technologies, a subtle modification (e.g. structurally, chemically, or electronically) near an interface can have a decisive effect on properties of the collective as well as each individual. A compelling case manifesting such subtlety is oxide heterostructures and heterointerfaces exhibiting fascinating emergent behaviours due to numerous combinative contributions of atomic structures and chemistries, which can be effectively harnessed for the design of advanced materials for information and energy applications and accelerating materials integration into advanced devices. Surface/interface X-ray scattering from modern synchrotron sources integrated with phase retrieval direct methods provides a very powerful toolkit to decipher the interfacial subtlety. This is essential to our ability to provide a quantitative and realistic description of the interfacial boundaries by which to engineer properties of functional interfaces using atomic structure-driven design principles in a reliable and controlled manner.

In this seminar, I will firstly give a brief introduction of how to obtain atomic mapping of multifunctional heterostructure and heterointerfaces with sub-Ångstrom resolution by phase retrieving coherent Bragg rods, wherein complete atomically structural information hidden, in particular on the COBRA method in combination with the difference map algorithm achieving unprecedented speed of convergence and precision. In the following, I will demonstrate some science cases in the exploration of oxide heterostructures and heterointerfaces for quantum information applications by applying the direct method, such as revealing structural motifs responsible for various quantum states (e.g. 2DEG/2DHG, interfacial superconductivity, polar metal and 2D skyrmions) adjacent with heterointerfaces, catching structural perturbations in response to internal and external electric fields, and depth-resolved mapping oxygen-octahedral connectivity network essential with incipient ferroelectricity of heterostructures. In the end, I will give a short commentary on emerging opportunities in X-ray studies of multifunctional interfaces and heterostructures of quantum materials enabled by the exciting advancements towards ultimate storage rings, in particular with enhanced high-energy, coherence and ultrafast capabilities.

Abstract ID: 992

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Invited Talk

Topics: Photonic devices and applications

Keywords: nanophotonics, low-dimensional nanostructures, III-V semiconductor materials, neuromorphic computing, spiking neural networks

Nanoscale light sources for neuromorphic nanophotonic circuits and computing

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Event-activated biological-inspired subwavelength optical neural networks are of key importance for future energy-efficient and high-bandwidth artificial intelligence (AI) systems. In this invited talk we outline the main challenges and our recent results towards the development of nanoscale light sources as key-enabling artificial spiking neurons for on-chip interconnected neuromorphic nanophotonic circuits. Neuromorphic nanophotonic circuit approaches as proposed here will significantly boost the transmission and processing capabilities of on-chip spike-based nano-optoelectronics for neuromorphic AI computing, offering exciting complementary solutions to electronics-based material solutions.

Abstract ID: 993

Symposium 2: Fabrication of Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Optical properties and spectroscopy of graphene and other two-dimensional materials

Keywords: MoS2 nanocrystallites, MoS2 natural single crystalls, graphene-like nanoparticles, Carbon additives, Raman spectra, graphite-like nanostructures, diamond-like nanostructures

Peculiarities of Raman Spectra of MoS2 Graphene-Like Nanoparticles with Small Carbon Additives

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A comparative study of the Raman spectra (RS) was carried out upon excitation by laser radiation of λL = 632.8 nm and 488 nm of natural molybdenite crystals 2H-MoS2 and CVD synthesized MoS2 (C) nanocrystallites containing 0.5 and 1.0 wt.% of carbon. A detailed numerical analysis of the shape of the observed D and G Raman bands was performed, including their decomposition into spectral components, as well as a comparison with the spectra of detonation nanodiamonds (~ 5 nm) and disordered graphite. The presence of vibrational bands of graphite-like (1330 – 1640 cm-1) and diamond-like (1168 – 1309 cm-1) structures has been established. All observed spectral components of carbon nanostructures and MoS2 are identified. A significant effect of resonance excitation of 632.8 nm on the electronic states and properties of MoS2 (C) nanocrystals was established. The enhancement of D bands of diamond-like structure and the ordering of the graphite structure with increasing of carbon content in MoS2 (C) nanocrystals have been established. The change in the frequencies of the D, G, and G(k) bands with an increase in the degree of disordering of diamond and graphite-like structures is considered. The effects of laser radiation on carbon structures are discussed.

Abstract ID: 994

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster/Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: Supercapacitor, Metal-Organic Framework, Zinc Sulfide, Solid State Gel Electrolyte, Nanoparticles

Zeolitic Imidazole Framework (ZIF-8) Derived Zinc Sulfide Nanoparticles for Energy Storage Application

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The increased industrialization and demand for renewable energy have inspired the research community to improve energy storage systems. From the last decade, the rise of the Metal-Organic Framework (MOF) has been proven to a revolutionary material for various applications. Herein, we have utilized ZIF-8 MOF to derive the ZnS nanoparticles through hydrothermal synthesis methods for energy storage applications. The obtained ZnS from ZIF-8 exhibit high crystallinity, high reaction sites, and nanoparticles confirmed from various characterization techniques including XRD, FESEM, and EDS. Further, the electrochemical testing has been done in the three electrochemical systems with 1M Na2SO4 electrolyte solution. The ZnS nanoparticles showed a capacitance of 190 F/g which can be attributed to the high surface area of the nanoparticles and redox activity. Additionally, the full symmetric solid-state supercapacitor device has been assembled with 1M Na2SO4 PVA electrolyte gel. The electrochemical device showed excellent electrochemical performance with long-term cyclability.

Abstract ID: 995

Symposium 3: Electronic, Photonic and Magnetic Materials (EPMM)

Oral Presentation

Topics: Nanomaterials and Nanotechnology

Keywords: nanobubbles, 2D materials, excitons, near-field imaging

Coupled nanobubbles in 2D lateral heterostructures

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Atomically flat semiconductors provide emerging platforms for new generation optoelectronic and quantum technologies. Nanobubbles in monolayer MoS2 and WS2 materials act as mesoscopic artificial atoms with exciton funnels generated by spatially engineered strain fields. We experimentally demonstrate near-field coupling of MoS2 and WS2 nanobubbles in a lateral 2D heterostructure, fabricated using high temperature superacid treatment, using far-field (FF) photoluminescence (PL) and near-field high resolution tip-enhanced photoluminescence (TEPL) nanoimaging. Due to the coupled plasmonic antenna, hot electrons and exciton funneling effects, we observe a synergistic enhancement in the PL and TEPL signals from different parts of the nanobubbles. We develop a theoretical model based on enhancement factors describing these various mechanisms, which shows a good agreement with experiments. The coupling of nanobubbles opens a new avenue for quantum information and exploration of nanodevices.

Abstract ID: 996

Symposium 1: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk

Topics: Artificial photosynthesis

Keywords: Nano-Bio Hybrids, Synthetic Biology, Energy Conversion, Hydrogen Evolution, CO2 reduction, value added chemicals

Merging Nanotechnology & Synthetic Biology toward Directed Evolution of Materials for Photocataysis

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The light-matter interaction has been making a major impact since the ignition and evolution of life on Earth. It is the cornerstone of modern life-changing technologies, above all, photocatalysis and sustainable energy production. In our work, we use a powerful combination of chemical synthesis, fabrication, and synthetic biology to develop hybrid hierarchical structures from atoms and molecules, resulting in new functions that go far beyond the individual starting components.

This talk will include recent examples of engineered nano-hybrid architectures based on light-gated natural proton pump either isolated from a host microorganism, or produced through cell-free synthetic biology. The fusion of a soft material, including a proton pump, with inorganic nanoparticles, or photonic supra-structures results in a functional "artificial cell" controlled by light. These hybrids demonstrate catalytic activities in H2 evolution reaction [1-4], CO2 reduction to value-added chemicals [5], and cell-mimicking synthesis of ATP [6].

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Abstract ID: 997

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Bio-inspired design of composites

Keywords: Carbon Nanotubes, Machine Learning, Nanolubricants

Machine learning approach for the nanolubricants design

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Carbon element displays an exceptional diversity of atomic 3D-arrangement-driven nanoarchitectures. The structures relying on C-sp2 hybridization are controllable and hence transferrable to macroscale materials of a one-of-a-kind combination of superb physico-chemical properties. One of the most intriguing phenomena observed for carbon nanoparticles as the tribo-active components and their formulations is called superlubricity. It can occur at the interface of a variety of tribo-pairs and results in the ultra-low, nearly vanishing friction coefficient (typically less than 0.01). Our tests confirm that he nanocarbons can reduce friction and wear in a spectacular way, even if simply added to the regular reference lubricants in such a low mass concentration as 0,01%, Fig. 1. Their mechanisms of tribological action are complex, multi-way and until now neither fully understood nor controlled. Here we propose machine learning-based modelling accompanied by molecular and supramolecular recognition toward understanding of the morphology and macro-assembling of multi-functional nanolubricants. The research was funded by National Science Centre, Poland, 2017/27/B/ST8/01838

Abstract ID: 998

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Composite structural materials

Keywords: Additive Manufacturing, Knee implant, Polymer, Biomedical, Mechanical Strength, Wear.

Evaluating the mechanical strength of the articulate component fabricated using the additive manufacturing process in the biomedical application

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Additive manufacturing is a layer-by-layer production technique which has been applied for different applications such as aerospace, automotive and biomedical application. In the biomedical field, especially the demand for knee implants is increasing worldwide due to arthritis problems. Furthermore, patient-specific implants are required because they will serve the patient reliably for a longer duration. The articulating component made up of polyethylene, attached to the femoral and tibial section experiences the most wear and bears the maximum load. Earlier, these components are developed by using the traditional technique like investment casting but lack structural integrity. Therefore, there is a need to fabricate the articulating components using a new technique like Fused Filament Fabrication (FFF) process, which allows us to increase the mechanical strength of the product by varying the process parameters such as layer thickness, infill density, printing speed and part orientation. The mechanical strength of the samples is evaluated by analyzing the compressive strength, wear-resistance, and fatigue strength of the polymer. The optimum parameters of the FFF process are selected based on the analysis and applied to the fabrication of the prototype (articulating component).

Abstract ID: 999
Symposium 4: Functional Composite Materials (FCM)
Oral Presentation
Topics: Smart Composites
Keywords: : Bracing system, Polyurethane, Self-centering, Experimental testing

Development of Novel Self-Centering Polyurethane Piston Based Bracing

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In braced frames, the response of a structure after an earthquake can be affected by the bracing system's strength and properties. Concentric Braced Frames (CBFs) are mostly used to resist the seismic load. However, traditional tension-compression bracing system may not perform well under earthquake loads because of buckling in compression. Other bracing systems such as Buckling Restrained Bracing (BRBs) and are being used to solve this problem. Buckling restrained braces are one of the practical systems to resist seismic loads. However, they cannot prevent permanent deformation in the building. To overcome the shortcomings of the developed system, a new Polyurethane Piston Based Bracing (PPBB) system has been developed and fabricated at the University of British Columbia. This device consists of a brace system that can take a considerable tension and compression force. The system is a cylinder-piston assembly in which polyurethane and steel are utilized. This specimen consists of five main parts: two halves of steel tubes, two polyurethane cylinders and a shaft. Quasi-static as well as strain rate experimental testing was performed on the device where very good self-centering behaviour was achieved using this relatively cheap and light material. This was achieved by analyzing the Displacement versus Force graph and finding the energy dissipation for this system.

Abstract ID: 1000

Symposium 4: Functional Composite Materials (FCM)

Oral Presentation

Topics: Industrial applications of composite materials

Keywords: calcium carbonate, composite filler, kaolin. silica, solid tire trolly

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Filler is one of the most important materials used to make various types of rubber vulcanizate. The filler in the rubber compound-making process acts as an active filler to improve the mechanical properties of the vulcanisate, and acts as a volume-increasing filler to reduce production costs. The filler composites used in this study are specifically for solid trolly tires which are commonly used to move goods within the airport area. Solid tire rubber vulcanisate in this study used a filler composite consisting of silica as an active filler, kaolin and CaCO3 as a volume enhancer. The loading of filler composites on the rubber matrix in this study varied from 50 to 65 phr. The manufacture of rubber composites for solid tires is carried out through a process of chewing, mixing natural rubber with synthetic rubber Butadiene Nitrile Rubber, componding, and vulcanization. The vulcanization process is carried out at a temperature of 150 °C for 20 minutes. The data from the test results before and after aging show that the composite filler ratio has an effect on specific gravity, hardness, and abrasion resistance. The homogeneity of the material was scanned using a scanning electron microscope (SEM). The scan results show that the distribution of the material on the rubber vulcanized matrix is influenced by the ratio of the filler materialTo see the functional groups of solid tire rubber vulcanisate used Fourier transform infrared spectroscopy (FTIR).

Abstract ID: 1001
Symposium 4: Functional Composite Materials (FCM)
Invited Talk
Topics: Green Composites
Keywords: Gelma, nanoliposome, functionalization

Nanofunctionalization of Gelatin Methacryloyl with Nanoliposomes

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Gelatin methacryloyl (GelMA) hydrogels have been widely used for various applications in the biomedical field, owing that to their tunable physicochemical and biological properties [1]. GelMA hydrogels allow cells to proliferate and spread due to the presence of cell-attaching and matrix metalloproteinase responsive peptide motifs, which makes GelMA mimic the native extracellular matrix (ECM) [2,3]. GelMA is a photocrosslinkable gelatin derivative produced by the substitution of the free amino groups with methacrylate anhydride. GelMA hydrogels showed better biological and physical properties when nanofunctionalized with hard or soft nanoparticles [4]. For biomedical use and because of their superior biocompatibility, soft nanoparticles are the preferred choice.

For this we nanofunctionalized GelMA with nanoliposomes that were produced by a low temperature enzymatic process developed by Linder et al. without the utilization of any chemical solvents [5]. Nanofunctionalized GelMA with nanoliposomes presented improved mechanical and physicochemical properties [6]. Moreover, nanoliposomes are composed of one or more lipid bilayer. Their amphiphilic nature allows them to increase the bioavailability of hydrophobic bioactive compounds and drugs by encapsulating them in the central core and protect hydrophilic bioactive compounds and drugs by encapsulating them in the lipid bilayer. This has been shown by the successful encapsulation of curcumin, which possesses poor water solubility and limited bioavailability, in nanoliposomes and by the increase in its solubility and bioavailability profiles [7,8]. Nanoliposome-encapsulated curcumin had a positive effect on the culture of primary cortical neurons by increasing their viability and network formation and decreasing their rate of apoptosis [7], and significantly increased MCF7 cancer cell cytotoxicity [8]. Furthermore, in addition to its antioxidant, anticarcinogenic, anti-inflammatory, antimicrobial properties [9], curcumin possesses immunomodulatory properties [10], which can prevent the inflammatory response of host immune cells towards hydrogel based scaffolds.