

Abstract ID: 101

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Plenary

Topics: Bio-inorganic nanomaterials

Keywords: gossypol; fluorescence polarization; ultraviolet method; fluorescent magnetic molecularly imprinted polymer

Preparation of Fluorescent Magnetic Molecularly Imprinted Polymer of Gossypol and Fluorescence Polarization Detection

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Fluorescent magnetic molecularly imprinted polymers of gossypol molecules were prepared and gossypol binding ability was detected by applying fluorescence polarization and ultraviolet methods. The experimental results showed that the fluorescent molecularly imprinted polymers had a high binding rate and high recognition ability of gossypol. Compared with the ultraviolet method, the fluorescence polarization method was more sensitive in evaluating the binding ability of molecularly imprinted polymers to gossypol. This is because the detection limit could be as low as 5ng/L and the linear range of detection was 5–45ng/L ($R^2 = 0.9958$). The preparation method of fluorescent magnetic molecularly imprinted polymers of gossypol was firstly discussed. It demonstrates that the fluorescence polarization applied in detection of molecularly imprinted polymers to gossypol is a sensitive and accurate detection method.

Abstract ID: 102

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Applications in orthopedic, cardiovascular, dental, nerve tissues, etc

Keywords: Carbon Nanotubes, Tissue Engineering, Hydroxyapatite

Carbon Nanotubes Reinforced Hydroxyapatite Based Functional Biomaterial for Regenerative Engineering

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Large bone defects caused by trauma, tumor resection, deformity, and infections are increasing year by year, but the rare resources for autogenous bone grafts and allograft rejections make it difficult to treat all of these deficiencies. In spite of high request in clinical medicine, nature's capability to self-organize the inorganic component with a preferred alignment in the bioorganic matrix is still not reproducible by synthetic techniques because of its complex nature. Therefore, in fields ranging from biology and chemistry to materials science and bioengineering a large developmental effort is essential in order to fabricate bone and dentin-like biocomposite materials, which may permit the ingrowth of hard tissues through improving mechanical properties with respect to the hard tissue regeneration.

In recent years, certain attention has been paid to biomimetic approaches, which allow us to mimic such natural bio-inorganic and bio-organic composite materials. The main idea in biomimetic methodologies is to control and fabricate the morphology and composition of developed biomaterials, in which the nano crystallites of inorganic compounds are spread with special orientation in the organic matrices due to its large potential in biomedical applications.

In the present work, we successfully mimicked electrospun bio-nanocomposite fibers on the basis of Poly Vinyl Alcohol (PVA) as matrix and Hydroxy Apatite (HA) nanoparticles with a highly anisotropic three-dimensional structure, microscopically the same as a substructure of bone. We have used two-step methodology that combines an in situ co-precipitation synthesis route with electrospinning process to prepare a unique type of biomimetic nanocomposite nanofibers of HA/PVA. The fibers produced by the electrospinning machine were in 100-200 nm. The result obtained from UTM analysis highlights the great tensile strength and young's modules of the nanofibers. A combination of structural, mechanical and biological properties of bone graft play a critical role in cell seeding, proliferation and new tissue formation in orthopaedic research. Nano-biomaterials should promote cell adhesion and be optimized for ECM production, mineralization and subsequent tissue regeneration. Hence, electrospun biomimetic HA/PVA/CNT nanofibers hold great potential for adhesion, proliferation and mineralization of osteoblasts and are favourable biocomposite scaffolds suitable for bone tissue redevelopment.

Abstract ID: 103

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Intelligent biomaterials

Keywords: Molecular-imprinting; Methamphetamine; Sulfonic acid resin; Chiral resolution

Chiral separation of (\pm)-methamphetamine racemate using molecularly imprinted sulfonic acid functionalized resin

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In the present study, a sulfonic acid functionalized enantio-selective resinous material was developed for effective chiral separation of (\pm)-methamphetamine racemate. R-methamphetamine-sulfonamide phenolic derivative was first prepared and fully characterized utilizing instrumental and spectroscopic techniques, then the sulfonamide was implemented in an acid catalyzed condensation copolymerization with phenol and formaldehyde. The resulted resinous material was then exposed to successive alkaline and acidic treatments in order to remove the R-methamphetamine enantiomer out of the resin matrix and obtaining the molecularly imprinted enantio-selective material, which was also investigated by scanning electron microscope, FTIR and XPS spectroscopy. The maximum selective extraction of the R-methamphetamine enantiomer was achieved at pH 7. The adsorption isotherms indicated an adsorption capacity of 233 ± 1 mg/g and followed the well-known Langmuir model. Also, the enantio-separation experiment of the racemic mixture was performed by column technique and both the supernatant loading and the eluant recovery solutions indicated an enantiomeric excess of 80% and 67% related to S- and R-methamphetamine, respectively.

Abstract ID: 104

Symposium 6: Functional Thin Films (FTF)

Invited Talk

Topics: Laser Resistant coatings

Keywords: laser, damage, film, semiconductor, transparent, electrode

Lifetime optical damage of wide bandgap semiconductor-based thin film transparent electrodes

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Wide bandgap materials are key materials in optoelectronic and power devices. Optimization of electrical, optical, and materials synthesis is a focus in industry and research in photovoltaics, display panels, energy efficient windows, flexible electronics, power electronics, and a range of other applications requiring low loss, good conductivity, and transparency in the Vis-NIR range. A new requirement for large aperture, high optical damage performance widegap materials is emerging to support the design of next generation optoelectronic devices suitable for compact, high rep rate, high power-handling laser systems. These requirements, sometimes-conflicting, necessitate selection of scalable, low defect semiconductor-based materials to go beyond the current optical damage limitations of typical conductive oxide, or second-generation semiconductor materials widely used in industry. In this study, a range of next generation widegap materials (GaN, SiC, α -Ga₂O₃, TiN) were tested to determine their optical damage mechanisms and lifetime performance. Intriguingly, this broad materials study suggests the possibility of using simple optical means to address power electronics materials in high power density applications. Additionally, we describe ways to engineer ruggedized widegap materials that are both less susceptible to absorption and thermally more stable, based on an understanding of the damage mechanisms involved in each type of material. Order of magnitude gains are demonstrated that can help establish a new class of widegap materials for high-power optoelectronics, power electronics industry, and for lasers used in high energy density research.

This work performed under the auspices of the U.S. DOE by LLNL under contract DE-AC52-07NA27344 within the LDRD program.

Wednesday, 21/Aug/2019 6:39pm - 6:54pm

Abstract ID: 105 / FBB-2: 14

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Invited Talk

Topics: Biomaterials for hard tissue applications

Keywords: Dental Caries, SAXS/WAXS, In Situ Analysis

In situ diagnosis of human enamel demineralisation using advanced time-resolved synchrotron X-ray techniques

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Dental caries is one of the most common chronic diseases that affect human teeth. It often initiates in enamel, undermining its mechanical function and structural integrity. The recent study has involved in situ quantification of the microstructure evolution over time in a simulated carious lesion. The aim is to collect insights into details of erosion during dental caries from the micro- to nano-scale to Ångstrom scale, with a view to learning to control it in ways that make maximum use of the natural remineralisation processes inside human oral cavity. This is the first in vitro and time-resolved investigation of enamel demineralisation using the advanced synchrotron X-ray techniques: small- and wide- angle X-ray scattering (SAXS and WAXS). From the analysis of experimental data it becomes apparent that the propagation of the erosion front is associated with not only the hydroxyapatite (HAp) dissolution, but also its re-precipitation. Moreover, we are able to observe that the crystal orientation of newly precipitated HAp particles differs from the preferred alignment characteristic (i.e. texture) of the particles in natural enamel. This study is likely to contribute to the understanding of the caries process and assist in developing effective therapeutic treatments to promote affected dental tissues to regain structural integrity.

Abstract ID: 106

Symposium 6: Functional Thin Films (FTF)

Invited Talk

Topics: Semiconductor and Superconductor film

Keywords: tetrathia/oxa[22]porphyrin(2.1.2.1)s, Charge transport, organic semiconductors, non-linear optics.

Functional organic materials: Synthesis and Structure dependent Charge transport and nonlinear optical behaviour of tetrathia/oxa[22]porphyrin(2.1.2.1)s and donor-acceptor dyads

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Nonlinear optical (NLO) responsive materials are of great interest for applications related to photonics, nanophotonics and optoelectronics, such as integrated optics, optical sensing, optical signal processing, optical computing, broad band optical communications, optical poling, optical limiting, etc. We recently investigated charge transport and NLO behaviour of tetrathia/oxa[22]porphyrin(2.1.2.1)s 1/2, which showed reverse saturable absorption at 527 nm, as a consequence of excited state absorption. We have now investigated nonlinear refraction, nonlinear absorption and two photon absorption at two different wavelengths using Z-scan method with nanosecond and femtosecond laser pulses. Complete characterization of the nonlinear optical behaviour of these systems shall be discussed.¹

In continuation with this, NLO behaviour of different designs of ferrocene (Fc) based donor-acceptor dyads 3-7 etc. have been investigated.^{2,4} The second-order nonlinear polarizabilities were determined using hyper-Rayleigh scattering (HRS) with femtosecond pulsed laser light at 840 nm. The dyads exhibit interesting structure-dependent NLO properties, which could be rationalized by correlating optical with electrochemical data.

Key Words: tetrathia/oxa[22]porphyrin(2.1.2.1)s, Charge transport, organic semiconductors, non-linear optics.

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Abstract ID: 107

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Novel 3D functional architectures consisting of low-dimensional nanomaterials

Keywords: N-doped Graphene, 3D hybrid, CVD synthesis

One-Step Synthesis of 3D N-doped Carbon Nanotube/N-doped Graphene Hybrid Material by Chemical Vapor Deposition

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A viable approach to achieving a robust 3D hybrid architecture is by integrating different low-dimensional nanostructures. The synthesis of three-dimensional carbon architectures from CNT and graphene effectively reduces the aggregation and stacking which occur among layers of graphene and CNTs. Nitrogen has smaller atomic radius and higher electronegativity than carbon and hence is a desirable dopant to improve electronic properties and surface wettability. We developed a facile one-step CVD technique approach to fabricate 3D N-CNTs/N-graphene nanomaterial using low-cost industrial melamine as a single carbon and nitrogen source (Figure 1). The N-CNTs/N-graphene are synthesized from one-dimensional N-doped carbon nanotubes and two-dimensional N-doped graphene which grown on the surface of nickel foam possessing interconnected porous 3D structure at 800 °C. The one-dimensional N-doped carbon nanotubes densely distribute on the surface of two-dimensional graphene sheet. The graphene sheet serves as supports of N-doped CNTs and Ni nanoparticles, which lead to nucleation and growth of CNTs and the CNTs in turn prevent the graphene sheets from aggregating. The results also show that defects appear in the wall of CNTs and graphene sheets, which means the successful nitrogen doping process of N-CNTs/N-graphene in the one-step CVD process. Remarkably, the atomic percent of nitrogen is up to 12.7%, which is higher than that of the previous reports on similar materials. And pyridinic-N is the main bonding configurations of nitrogen atoms in the 3D hybrids. The doped nitrogen induces more defects and active sites on the surface of carbon framework but also effectively improves the electronic properties and surface wettability. This study offers a promising route to produce the functional N-CNTs/N-graphene nano-architecture.

Abstract ID: 108

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Design and application of composite structures

Keywords: Zinc oxide nanoparticles, Graphene, Nitrophenol, Square wave adsorptive stripping Voltammetry.

An electrochemical sensor based on graphene nanosheets-zinc oxide composite coated glassy carbon electrode for the sensitive determination of para-nitrophenol

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Graphene and graphene oxide carbon materials have attracted a great deal of attention for sensing applications due to their excellent charge transfer mobility, large specific surface area and good electrocatalytic activity^{1,2}. Recently, one new perspective is to utilize ideal single-atom-thick GN as a support to anchor functional nanomaterials to form new nanocomposite with potential application^{2,3}. On the other hand, there is no report in the literature for the electrochemical determination of para-nitrophenol (p-NP) using graphene nanosheets-zinc oxide nanoparticles (GNS/ZnONPs) based composite as sensing material. In the present study, ZnONPs have been synthesized by wet chemical method and have been dispersed with graphene oxide (GO) for the fabrication of GNS/ZnONPs composite using glucose as reducing agent. Reduction of GO to GNS and anchoring of ZnONPs on GNS have been simultaneously achieved. The materials were characterized using X-ray diffraction, scanning and transmission electron microscopy, Raman and energy dispersive X-ray spectroscopy. Electrode characterizations were carried out using electrochemical impedance spectroscopy, chronocoulometry and cyclic voltammetry (CV). The GNS/ZnO nanocomposite was used as a modifier for glassy carbon electrode (GCE) by depositing the composite onto GCE using drop deposition method. The modified electrode has been applied for the determination of (p-NP) using voltammetric techniques. The good dispersion of ZnO nanoparticles with GNS showed enhanced electrocatalytic activity towards the electrode reduction of (p-NP) compared with individual GNS modified GCE in 0.1M phosphate buffer (pH 6.8) using CV. A wide linear working range of 9.90×10^{-8} M to 2.18×10^{-6} M and detection limit of 8.8×10^{-9} M using square wave adsorptive stripping voltammetry was obtained. Both ortho and para-nitrophenols can be detected simultaneously at the developed electrode in presence of meta-nitrophenol without the interference. The proposed method was applied to determine p-NP in river and ground water samples with satisfactory recoveries.

Abstract ID: 109

Symposium 2: Functional Composite Materials (FCM)

Invited Talk

Topics: Design and application of composite structures

Keywords: Electrochemical techniques, Sensors, Nanocomposites, Environment, energy density.

Advances in electrochemical sciences: new approaches to environmental applications involving functionalized novel nanomaterials

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Recent advancement in the field of electrochemical sciences and nanotechnology has shown that advanced functional nanomaterials play an increasing role in environmental monitoring. The combination of nanotechnology and modern electrochemical techniques allows the introduction of reliable and powerful electrochemical devices for environmental applications.

Two major environmental issues that everybody is facing nowadays is the environmental pollution of some important substances (CN-1, NO₂-1, NO₃-1, SO₃-1, some toxic metals, pesticides, insecticides, polycyclic hydrocarbons, etc) and the need of low-cost, environmental-friendly and high-performance energy storage devices known as supercapacitors. These two issues have been taken into consideration simultaneously in this lecture because both the problems can have a common solution. The same electrode material can be used as a selective and sensitive detector as well as an efficient electrode material for energy storage applications in supercapacitors.

Our group has designed some electrodes based on advanced functionalized materials which find potential applications for the sensitive detection of environmentally hazardous substances and some electrodes were fabricated and investigated for their performance in energy storage applications in supercapacitors.

I shall exemplify our new approaches for the synthesis of some advanced functional materials based on metal nanoparticles, metal porous oxides and polymers with carbon based materials (graphene and graphene oxide). Applications of these materials for the sensitive detection of metal toxicity, nitrophenols and pesticides in various environmental samples will be discussed in the lecture. In addition, some novel nanocomposite material functionalized electrodes and their applications in energy storage devices (supercapacitors) will also be exemplified.

Abstract ID: 110

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biomaterial surfaces

Keywords: silica, sol-gel, DNA, ROS, melatonin

Influence of melatonin on sol-to-gel transformation of DNA encapsulating silica: Barrier against ROS damage

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Today, development of novel materials to carry and shield nucleic acids against several hazards is a challenging, yet imperative task for gene transfer, silencing or biosensor applications. In current methods, carrier materials are produced first, and then nucleic acids are loaded onto materials by physical or chemical interactions. Being the number-one nontoxic candidate for gene silencing research, mesoporous silica particles have shown a great oligo delivery potential together with immediate concerns on protection of nucleic acid conformation and prevention of pre-release [1]. In this work, DNA oligonucleotides were encapsulated in plain and melatonin loaded silica upon sol-to-gel transformation. By the hydrous sol-gel method followed in this work, DNA conformation could be shielded from degradation by encapsulation in deep, interconnected mesopores without using complex procedures or sacrificing from biocompatibility. Influence of melatonin, a key anti-cancer agent with oncostatic activity, on DNA encapsulated silica structure and ROS (hydroxyls ($\bullet\text{OH}$), alkoxy radicals ($\text{RO}\bullet$), etc.) damage resistance was investigated using Fourier Transform infrared (FTIR), ^{13}C and ^{29}Si nuclear magnetic resonance (NMR) spectroscopy, differential scanning calorimetry (DSC), X-ray diffraction (XRD), gas adsorption and high-resolution transmission electron microscopy (HR-TEM). The biocompatibility of the particles was investigated by in-vitro cytotoxicity analysis using MTT assay. The kinetics of DNA release from melatonin/silica particles was determined by measuring the change in specific UV absorption of DNA at 230, 260 and 280 nm, in RNase free water at specific time periods (1-24 h) and varying pH (2,7 and 9). ROS damage resistance of DNA encapsulating melatonin/silica particles were investigated by exposing particles to Fenton's reagent and observing the change in encapsulated DNA conformation by spectroscopy. Results showed that melatonin incorporation into gelling silica did not cause phase separation, toxicity or inhibit DNA encapsulation. DNA release rate, silanol content (Si-OH; hydroxyl binding uncondensed silica species) and porosity of the amorphous network were influenced by melatonin incorporation (0-20 mg/mL), however it did not disturb the native conformation of DNA. Considering that aging and various diseases are caused by ROS, their interactions with nucleic acids and additive effect of melatonin on the efficacy of anti-cancer drugs [2], this study is the first to show the potential of biocompatible melatonin/silica composites for oligo/drug delivery and biosensor applications.

Abstract ID: 112

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Hybrid cells for energy harvesting

Keywords: liquid Zn-Ferrum batteries, high efficiency, energy density, reliability

Zinc ferrum energy storage chemistries with high efficiency and long cycling life

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Energy storage systems with higher energy density and good electrochemical performance are the urgent demand in new energy industry for electric vehicles. Rechargeable aqueous Zn-ion batteries (ZIBs) are particularly attractive owing to the safety, nontoxicity, inexpensiveness and high energy density. Here, we propose a new prototype of liquid Zn-Ferrum batteries (ZFBs) using metal Zinc as anode and aqueous Fe(II/III) redox couple as catholyte. This battery presents excellent electrochemical performance with the capacity of 352 mAh g⁻¹ at an average discharge voltage up to 1.25 V, an energy density of 391 Wh kg⁻¹, a power density of 2.2 kW kg⁻¹ at current density of 2 A g⁻¹, and long cycling life: no evident capacity fading after 5000 cycles. In the case of the ZFBs system, sub-nanometer pores of CF-N-O enable low self-discharge rate via Fe²⁺ and Fe³⁺ adsorption in carbon nanopores, which was achieved without applying an ion exchange membrane. It was testified as a promising energy storage system with high efficiency, energy density, reliability and durability, and it might be a promising application in electric vehicles.

Wednesday, 21/Aug/2019 6:24pm - 6:36pm

Abstract ID: 113 / FBB: 13

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Drug delivery/controlled release

Keywords: nanomedicine, drug delivery, in vivo, zebrafish

Zebrafish embryos as a tool to study the in vivo behavior of nanomedicines

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Nanomedicines are the most promising method for delivering sensitive or toxic therapeutics in a cell or tissue selective manner. Through nanocarrier encapsulation and/or conjugation, the pharmacokinetics (e.g. bioavailability) and/or tissue distribution of drugs within the body can be modified. Yet despite this huge effort and investment, there are currently just a few antibody-drug conjugates (ADCs) and nanoparticle-based therapies on the market. This low success rate clearly demonstrates nanomedicines have a delivery problem. Typically less than 1% of administered nanomedicines reach their intended target in the body and there has been no significant technological advance to improve these meagre targeting efficiencies over the past 30 years. Zebrafish (embryos) are increasingly used as model organisms to study fundamental biological processes (e.g. embryogenesis and disease pathogenesis). Their transparency enables high resolution light microscopy imaging of these processes across entire organisms and in real time, and (fluorescent) transgenic lines are readily available.

To validate the zebrafish model as a new in vivo tool for the field of nanomedicine, we recently screened >50 liposome formulations, both experimental and clinically relevant, in zebrafish embryos to assess the influence of lipid composition on in vivo liposome fate. This study showed that zebrafish are an accurate tool to assess, quantify, dissect and exploit nanomedicine fate at (sub)cellular resolution and across whole living organisms (i.e. accounting for the total injected dose). Our discovery of scavenging endothelial cells (SECs) in the embryonic zebrafish is the earliest developmental stage at which these cells have been identified in any vertebrate. Genetically and functionally analogous to liver sinusoidal endothelial cells (LSECs) in mammals, we were able to show anionic liposomes were taken up by SECs exclusively via the scavenger receptor, stabilin-2. This we believe represents a major off-target of many clinically approved nanomedicines. Importantly, we also showed that the observed in vivo behavior of liposomes in embryonic zebrafish was conserved in a mammalian (adult mouse) model. In this presentation I will present our recent results on how lipid composition influences in vivo fate of liposomes/lipid nanoparticles and how a synthetic fusion system aids in the cell-specific uptake.

Key Words: Nanomedicine, Drug delivery, Zebrafish, In vivo

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Abstract ID: 114

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Additive manufacturing Applications

Keywords: Poly(vinylidene) fluoride, electroactive response, carbon nanotubes, nanofiber generator

Hybridizing SWNT/PMMA/PVDF towards High-Performance Piezoelectric Nanofibers

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Piezoelectric nanofibers are of great importance in their potential applications as smart fibers and textiles to bring changes to daily lives. By employing the technique of electrospinning, nanofibers of PVDF modified with polymethyl methacrylate (PMMA) and single-wall carbon nanotubes (CNT) (referred to as CNT/PMMA/PVDF) are prepared. The electric field induced displacement of the as-prepared nanofibers is characterized by a Piezoresponse Force Microscope (PFM). Compared with the pure PVDF nanofibers, nanofibers of CNT/PMMA/PVDF exhibit a great enhancement of about 196 % for the electric field induced displacement, while increments of about 104 % and 78 % are obtained for nanofibers of PMMA/PVDF and CNT/PVDF, respectively. Structure analysis indicates that the hydrogen bonding between the O atom in carbonyl group of PMMA and hydrogen atom in CH₂ groups of PVDF, promotion of crystallites nucleation by CNT, work synergistically to produce the high electroactive response of the nanofibers of CNT/PMMA/PVDF. Based on the high-performance nanofibers, a prototype of flexible nanofiber generator is fabricated, which exhibits a typical electrical output of 3.11 V upon a repeated impact-release loading at a frequency of 50 Hz.

Abstract ID: 115

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Synthesis, Characterization and modeling of the atomic processes of bulk and thin-film oxide film formation

Keywords: Calcium Sulphide, Scalar wave Thin Film, Dielectric Perturbation, Wave Propagation Solid State and Optical Properties

Theoretical Approach to Study the Solid State and Optical Characteristics of calcium Sulphide[CaS] Thin Film.

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Calcium sulphide thin film has been studied in this work using theoretical approach in which a scalar wave is propagated through the material thin film deposited on a glass substrate with the assumption that the dielectric medium has homogenous reference dielectric constant term, and a perturbed dielectric function, representing the deposited thin film medium on surface of the glass substrate is presented in this work. These two terms, constituted arbitrary complex dielectric terms that describes dielectric perturbation imposed by the medium of for the system. This is substituted into a defined scalar wave equation in which the appropriate Green's Function in conjunction Dyson's equation was defined on it to reduce it to Volterra equation of second type with the kernel is solved using series solution technique in conjunction with Born approximation method in order to obtain a model equation of wave propagating through the thin film. This was used in computing the propagated field, for different input regions of field wavelength such as ultraviolet, visible and infrared region respectively during which the influence of the dielectric constants of the thin film on the propagating field were considered. The results obtained from the computed field were used in turn to compute the band gaps, solid state and optical properties of the thin film such as reflectance, Transmittance and absorbance.

Abstract ID: 116

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Applications of Biopolymer for Drug Delivery

Keywords: biodegradable nanofiber, anti-adhesive membrane, sustainable release, lidocaine, ketorolac

Analgesics Embedded Biodegradable Nanofibrous Anti-adhesive Films Providing Sustainable Pain Relief for Surgical Wounds

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This study developed and evaluated the effectiveness of biodegradable, nanofibrous lidocaine/ketorolac-loaded anti-adhesion nanofibers to sustainably release analgesic at abdominal surgical wounds. The analgesics-eluting membranes of two polymer-to-drug ratios (6:1 and 4:1) were produced via an electrospinning technique. A high performance liquid chromatograph (HPLC) assay was employed to characterize the in-vivo and in-vitro release behaviors of the pharmaceuticals from the membranes. It was found that all biodegradable anti-adhesion nanofibers released effective concentrations of lidocaine and ketorolac for over 20 days post-operation. In addition, a transverse laparotomy was set-up in a rat model for an in vivo assessment of activity of post-operative recovery. No tissue adhesion was observed at two weeks post surgery, demonstrating the potential anti-adhesion capability of the drug-eluting nanofibrous membrane. The post-operative activities were recorded for two groups of rats given below: rats that did not have any membrane implanted (group A) and rats that had the analgesics-eluting membrane implanted (group B). Rats in group B exhibited faster recovery times than those in group A in regards to post-operative activities, confirming the pain relief effectiveness of the lidocaine and ketorolac-loaded nanofibrous membranes. The experimental results suggested that the anti-adhesion nanofibrous membranes with sustainable elution of lidocaine and ketorolac are adequately effective and durable for the purposes of post-operative pain relief in rats.

Abstract ID: 117

Symposium 2: 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.

Thursday, 22/Aug/2019 11:00am - 11:12am

Abstract ID: 118 / FCM-3: 1

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Biocomposites

Keywords: microspheres, polymer films, composites, gelatin, starch, sodium alginate

Modification of sodium alginate/starch films by addition of microspheres

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The synthesis and characteristics of polymer microspheres are the subject of numerous studies. The last decade has been characterized by the extremely rapid development of microparticulate systems used in many branches of science, especially in medicine, pharmacy and cosmetics [1-3]. The aim of this paper is to obtain composite materials for cosmetic or dermatological applications by means of incorporating polymer microparticles (containing plant extract) in the polymer matrix. Due to the fact that these materials should be characterized by biocompatibility and non-toxicity, the biopolymers, such as gelatin, sodium alginate and starch, which are known for their unique properties suited to medical applications, were used in this study. Gelatin microspheres were prepared by an emulsification/crosslinking method [4]. In the next step, microspheres were incorporated into a sodium alginate/starch thin matrix. The morphology and size of the microparticles, as well as the morphology, swelling properties, mechanical properties, and stability of microsphere-loaded films were measured. This novel delivery system was tested to control the release of *Calendula officinalis* flower extract. This study offers a promising material for biomedical or cosmetic applications.

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Acknowledgments

Financial support from National Science Centre (NCN, Poland) Grant no. UMO-2016/21/D/ST8/01705 is gratefully acknowledged.

Abstract ID: 119

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biomaterial surfaces

Keywords: Key Words Novel synthetic route, Chitosan, nanofibers membrane, Bio-adsorbent, Enhanced metal ions removal

Novel Route for Amine Grafting to Chitosan Electrospun Nanofibers Membrane for the Removal of Copper and Lead ions from aqueous medium

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A novel step wise synthetic route was used to prepare amine grafted nanofibers (AGNFs) affinity membrane. The chemical structure of the nanofibers (NFs) after grafting was studied by acquiring Fourier Transform Infrared (FT-IR) spectra and Carbon, Hydrogen and Nitrogen (CHN) data. The morphology of the NFs before and after grafting was studied by Field Emission Scanning Electron Microscope (FE-SEM). FT-IR and CHN data confirmed the introduction of new functional groups into the primary structure of chitosan (CH). FE-SEM showed denser membrane with no deterioration of the NFs morphology after grafting. The aqueous stability of the membranes was studied in distilled water. The AGNFs membranes showed good aqueous stabilities (with only ~ 6% loss in weight until 24 h and remained stable thereafter) which was less than the weight loss by glutaraldehyde treated nanofibers (GNFs) (~44% loss in weight until 24 h) and NFs (100% loss in weight as soon after it was immersed in distilled water). The maximum adsorption (qm) capacity of AGNFs for Cu (II) and Pb (II) was observed to be 166.67 mg.g-1 and 94.34 mg.g-1. The adsorption capacity of the present systems was much higher for Cu (II) when compared to the already existing conventional and chitosan adsorbents. This increased might be related not just to the size, but more potentially to the increase in the number of nitrogen binding sites (chelating sites). Nitrogen donates lone-pair of electron for chelation. The combination of processing and amine grafting (AG) significantly increased the adsorption capacity of NFs membranes.

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Thursday, 22/Aug/2019 3:03pm - 3:15pm

Abstract ID: 120 / FLNM-3: 6

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Applications of low dimensional, nano and 2D materials

Keywords: Graphene, Functionalization, Heterostructures, Dynamic Covalent Motion

Chemistry on and with Graphene: Introducing Selectivity, Functionality and Motion

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Reaching the ultimate potential of graphene in multitude of fields requires means of on-demand tuning of its properties. Covalent chemical functionalization of the graphene monolayer provides merely unlimited space for targeted attachment of various moieties and thus manipulation of intrinsic parameters of the material. The approach, however, is facing three crucial challenges on the way towards its goal: achieving the chemical reaction, characterizing its products, and application of the chemical functional group in extending functionality of the material.

The covalent modification of graphene can now be realized by three mechanistically different approaches, by i) radical, ii) nucleophilic or iii) electrophilic.[1,2] This is crucial to overcome incompatibilities of functional groups with the grafting protocol. The characterization of 2D materials, traditionally dominated by Raman and XPS, provides only limited insight into the surface chemistry. Successful application of other methods, including MS, SERS or IR has been demonstrated, [1,3,4] thus completing the structural information about the monolayer.

The introduced moieties modulate the electronic structure of graphene, e.g. Fermi level, which consequently tune the efficiency of graphene-enhanced Raman scattering.[5] The grafted groups also bring new functionalities, such as sulfonyl groups on graphene serving as the catalyst and stabilizing layer for selective polymerization of PEDOT.[6] Patterning of graphene provides selective formation of perovskite heterostructures with superb spatial resolution.[7] Finally, covalently dynamic bonds can be envisaged, allowing for thermodynamically controlled connectivity and out-of-equilibrium manipulation with species on the nanoscale.[8]

Key Words: Graphene, Functionalization, Heterostructures, Dynamic Covalent Motion

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Abstract ID: 121**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)****Invited Talk**

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

Keywords: Nano Energy Storage, Fast-ion-conductor, SOFC, Upconversion Luminescence

Probing oxide-ion conduction in low-temperature SOFCs**Bolong Huang**

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Driven by the fierce power issues, by no means fortuitous, Solid Oxide Fuel Cells (SOFCs) has arisen to be a competitive candidate because it no needs charging to initiate operation and exhibits environmental benignity and high energy efficiency (easily levels up to 40~60% or even 70%). They do not necessarily follow Carnot-Cycle thermodynamic Law, and only rely on a fast redox reaction predominantly fed by O₂ or oxidizing agent. The in-system bio-circulating regenerative SOFCs have gradually aroused our attention, as it indeed serves as the embedded inclusion type renewable electrical generations. It has been recently applied in the deep-space exploration aircraft of China called "Lunar-Palace-One-Project". This project results from their ability to optimally support the biologic internal recycle system and supply enough energy for living needs of astronauts at environment of moon, which can be attributed to recent outstanding progress on oxygen storage materials for electrodes, catalysts with high efficiency for oxygen/hydrogen generation and fast ion conductors. As a challenge, fast ion transportation with electronically insulated will decrease the voltage loss and further determine the electrical performance, which usually could only be ensured in high working temperature. Moreover, most ordinary SOFCs have rather high working temperature at least above 800°C. Screening and characterizing the candidate electrolyte onsets in lower temperature without sacrificing electrical performance, become urgent. It is worthy considering that this demanding in-situ screening and characterization under such high dynamic temperature cannot be fulfilled by current technique.

Herein we report an in-situ and non-contact method to monitor the working condition of solid oxide fuel cells (SOFCs). With the combination of density functional theory calculation and upconversion (UC) luminescence, we give distinct and complementary perspective on the entangled interaction between thermal-driven formed O-ion Frenkel pair (native solubilizer) and Bi³⁺ dopant (competitive inhibitor) in La₂Mo₂O₉ derivatives, especially at a lower temperature required by a SOFCs device. As we know, innovating higher electrical performance at lower temperature mainly depends on the screening of the candidate electrolytes. The thermally driven formation of a-Fr pairs has been believed to be the initiation of ion conduction, which has rarely been investigated. Generally, only with certain amount of a-Fr pairs formed in lattice, ion conduction could be probed by equipment. However, this in-situ non-contact luminescence method supply a new reliable way of monitoring the complete process of a-Fr pairs formation and ion conduction with corporation of DFT calculations. This is important for thoroughly understanding the ion conduction mechanism and will further benefit controlling properties of materials to realize high conductivity in low temperature.

Thursday, 22/Aug/2019 3:12pm - 3:27pm

Abstract ID: 122 / FESC-2: 7

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

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

Keywords: Nanogenerators, Piezo-phototronics, Energy conversions, Native defects.

Intrinsic energy conversions for photon-generation in piezo-phototronic materials: A case study on alkaline niobates

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The creations of photons in response to mechanical stimulus in a crystal that has noncentral symmetry are the great fundamental physics responsible for numbers of important technologies. The underlying mechanism and complete theory for a precise explanation of the mechanical-photonic energy conversion phenomena is vital important. We take commercial piezoelectric LiNbO₃ matrices as the example to interpret the detail mechanisms of energy conversions for the photon-generation through a native point defects study. It was found the Frenkel and Schottky type complex pairs as well as the antisite pair defects acting as energy harvesting and migration centers, which are very easy to form and active. It does to be the extra deep electron or hole traps levels near the valence or conduction band edge, respectively. That is the substantial energy reduction via a spontaneous equilibrium transformation from the complementarily charged individuals into agglomerated complexes. Such energy gain for both two processes turns to be independent to the variations of synthesis chemical potentials. In addition, the complex defects actually form independent to the variations of the chemical potentials. This leads to a coupling and exchange effect by them to continuously collect and transport host charges along the path via localized states to the deep recombination levels. The initiating energy barrier is small which ambient thermal stimulation or quantum tunneling can accomplish. The native sensitizers such as VNb₂O₅, VLiNbO₃, NbLi are also the energy conversion centers to non-radiative resonant energy transfer onto the activator center at the O_i to transfer the energy into photon emissions. A generalized energy conversion mechanism has been unraveled in this work. This gives a solid theoretical reference for developing the mechanical-photonic energy conversion materials.

Abstract ID: 123

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin Films in Biological and environmental Applications

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

Palladium (II) Oxide Nanostructures for Detection of Ozone and Nitrogen Dioxide in Ambient Air

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Low level ozone is a product of industrial production, transportation and other activities leading to unwanted air pollution. Ozone accumulates at the surface of the Earth and the process has accelerated in the last twenty years. Air pollution with ozone and nitrogen dioxide is a serious problem owing also to cyclic processes of these gases mutual transformation under sunlight [1]. Interaction of O₃ and NO₂ with volatile hydrocarbons produces within oxidation reactions many toxic organic substances. Organizations such as WHO and US EPA declared that ozone and nitrogen dioxide can be very dangerous for human health, particularly for children, the elderly, and people who have lung diseases [2].

Various wide band gap metal-oxide semiconductors are studied as gas sensing materials for detection of these toxic gases. Palladium (II) oxide nanostructures have been employed for O₃ and NO₂ detection [3, 4]. Homogeneous thin and ultrathin PdO films with p-type conductivity and energy band gap $\Delta E_g = 2.3$ eV were prepared on polished poly-Al₂O₃, SiO₂/Si (100), optical quality quartz, and amorphous carbon/KCl substrates. PdO films were obtained by thermal oxidation in dry oxygen at temperatures $T = 670 - 870$ K of pure palladium layers. Homogeneous PdO films prepared at $T = 870$ K were tested for detection of nitrogen dioxide and ozone. They demonstrated excellent values of sensitivity, signal stability, recovery time, operation speed, and reproducibility of sensor response. Preparation of PdO films is simple and they can be easily integrated into microelectronic devices. PdO nanostructures show also other important advantages when compared to different materials currently used for gas sensors fabrication [4].

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Abstract ID: 124

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Electrode/electrolyte interface phenomena

Keywords: Polypyrrole, Paratacamite, Electrochemical analysis, Hydrogen storage.

Inorganic Mineral Doped Polypyrrole for Hydrogen Storage in Alkaline Medium

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Paratacamite doped Polypyrrole was synthesized by wet chemical method employing CuCl_2 as oxidant. The transitions of doped polypyrrole polaron-bipolaron states were analysed by Raman spectroscopy. Electrochemical analysis of Paratacamite doped Polypyrrole in 0.01M NaOH indicated hydrogen storage ability and evolution kinetics. Heterogeneous rate constant was calculated from cyclic voltammetry. The maximum charge stored as protons in the Paratacamite doped Polypyrrole is 16F/g calculated from linear sweep voltammetry at lower scanrate.

Abstract ID: 125

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: supercapacitor, electrode materials, LaMnO₃, nanocomposite

LaMnO₃@NiCo₂O₄ Nanoarchitecture for High Performance Supercapacitors

Hongwei Tian¹, Xueqin Lang¹, Haoshan Nan², Xiaoying Hu²

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The effective composited materials with structural optimization have potential for improving the electrochemical performance of supercapacitors in recent years. Herein, we put forward a rational design to fabricate LaMnO₃@NiCo₂O₄ core-shell architectures composed of nanosheets on Ni foam substrate by facile hydrothermal processing. Owing to the synergistic contribution between LaMnO₃ nanoparticles and the porous nanosheets of NiCo₂O₄, the hierarchical electrodes with high oxygen vacancies achieved remarkable electrochemical performances with a wide potential window (-0.8-0.6 V). This makes such hybrid structure possess a high specific capacitance of 812.5 F/g at 0.5 A/g with capacitance retention of 73% after 10000 cycles at high current density of 20 A/g and nearly 100% coulombic efficiency in 6 M KOH electrolyte. It is noteworthy that the energy density of the asymmetric supercapacitor with activated carbon (AC) as the negative electrode is 44.7 Wh/kg at a power density of 750 W/kg, while the LaMnO₃@NiCo₂O₄ material as the positive electrode. The impressive results suggest that LaMnO₃@NiCo₂O₄ can be a promising electrode material for supercapacitor applications.

Abstract ID: 126**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Photocatalytic and electrochemical water splitting

Keywords: Water splitting, acidic electrolyte, manganese oxide, potential window

Stable Potential Window of Transition Metal Oxides for Efficient and Stable Oxygen Evolution Reactions in Acidic Electrolyte**Hongxian Han**

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Artificial photosynthesis of solar fuels, such as hydrogen production via water splitting driven by solar energy, is an ideal solution for the sustainability of energy supply. Oxygen evolution reaction (OER) is considered to be the key primary step for achieving overall water splitting. Water oxidation reaction generates reductive electrons and H⁺ while deliberating gaseous molecular oxygen. The production of H⁺ makes the vicinity of water oxidation catalyst in acidic environment if these protons are not quickly consumed or transferred far away. The micro-acidic environment requires development of OER catalyst that is not only efficient but also acid-tolerant.¹

At present, the only well-established electrocatalysts for the oxygen evolution reaction (OER: 2H₂O → O₂ + 4H⁺ + 4e⁻) are the oxides derived from iridium (Ir) under proton exchange membrane (PEM) acidic environment. Considering that the employment of PEM electrolyzers for water splitting at TW scale would require over ten years of Ir production, the development of acid-stable non-noble OER catalysts is the most important challenge.²

In this talk, I will present our recent research progress in the development of acid-stable transition-metal based OER catalysts. Typically, it was found that γ-MnO₂ with intergrowth of pyrolusite (β-MnO₂) and ramsdellite (R-MnO₂) phases, can catalyze the OER for over 6000 hrs at 10 mA cm⁻² with a specific potential of 1.65-1.75 V in a pH 2 electrolyte. This is more than 100 times longer than any other earth-abundant metal oxides reported so far. The voltage efficiency of γ-MnO₂ in an electrolyzer with a PEM was 70.12% at room temperature, showcasing how a material traditionally perceived to be unstable in acid has potential application as an industrial OER catalyst.³

This system is still operating today, showing the importance of precisely regulating electrochemical conditions with respect to the stable potential window. At the system scale, we expect that such potential windows are highly synergetic for water electrolysis using renewable electricity such as solar and wind energy. The spectroelectrochemical approach of identifying stable potential windows can readily be applied to other earth abundant metals such as Fe, Co, and Ni, paving the way toward noble-metal-free PEM systems which can operate in the timescale of years.

Acknowledgement

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Thursday, 22/Aug/2019 12:12pm - 12:24pm

Abstract ID: 127 / FTF: 7

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Advances in Deposition Techniques for thin films

Keywords: Germanium-antimony-telluride, Chemical vapor deposition, Atomic layer deposition, Precursors

Molecular Precursors for the Phase-Change Material Germanium-Antimony-Telluride, Ge₂Sb₂Te₅ (GST)

Nicole Harmgarth, Florian Zörner, Phil Liebing, Edmund P. Burte, Mindaugas Silinskas, Felix Engelhardt, Frank T. Edelmann

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This lecture intends to provide an overview of the precursor chemistry that has been developed around the phase-change material germanium-antimony-telluride, Ge₂Sb₂Te₅ (GST). GST is a promising material for the construction of non-volatile memory cells for use in modern microelectronics. Thin films of GST can be deposited by employing either chemical vapor deposition (CVD) or atomic layer deposition (ALD) techniques. In both cases, the success of the layer deposition crucially depends on the proper choice of suitable molecular precursors. Previously reported processes mainly relied on simple alkoxides, alkyls, amides and halides of germanium, antimony, and tellurium. More sophisticated precursor design in our lab has now provided several new sets of volatile molecular precursors of Ge, Sb, and Te, including unprecedented aziridinides (Figure 1a), new amidinates (cf. Figure 1b), and liquid dialkylditellurides such as nBuTeTenBu (Figure 1c). Most of these compounds were structurally characterized through single-crystal X-ray diffraction. The new precursors have been successfully employed for the plasma-assisted ALD (PALD) of smooth and uniform films of GST. Even complex structures such as holes and grooves could be filled and covered by GST layers (cf. Figure 1d).

Abstract ID: 128

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Exfoliation and unzipping 2D materials

Keywords: Graphene, Carbon dots, Direct exfoliation, Ultrasonication

Direct Exfoliation of Graphite from Carbon dots derived from Cannabis Sativa

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Liquid phase exfoliations of Graphite (Gr) to Graphene (G) were initially done using modified hummers method.¹ Hydrophobic nature of G limits its applicability especially in different biomedical applications. Herein, C-dots can become a suitable candidate to directly exfoliate Gr to G. Jiang et al., demonstrated graphene quantum dots can act as stabilizer for aqueous dispersion of G with good stability.² Exfoliation of Gr using C-dots is in infant stage as citric acid was used as a sole carbon precursor.³ Herein, in present work for the first time “Cannabis Sativa” was used as green carbon source to fabricate nitrogen doped C-dots (N@CSDs) to directly exfoliate Gr to G (GN@CSDs). The optical properties of N@CSDs were studied using absorption and fluorescence spectra. The absorption peak around 280nm corresponds π - π^* transition. The fluorescence spectra of N@CSDs exhibit wavelength tuned emission behaviour. The synthesized N@CSDs showed spherical morphology. N@CSDs exhibit horizontal distance in the range 12.5-13.5nm and vertical distance less than 1.5nm. To confirm the successful exfoliation Raman spectra of GN@CSDs (Fig. 2a) were recorded. The 2D peaks of GN@CSDs were deconvoluted in the range 2550-2700 cm^{-1} (Fig. 2b) into 4 components. Two major peaks were appeared at 2600 & 2635 cm^{-1} and two minor peaks were at 2570 & 2660 cm^{-1} . GN@CSDs shows signature absorbance peak around 280nm (Fig. 2c) arising from π - π^* transition. Fluorescence measurement shows quenching in the fluorescence intensity of N@CSDs w.r.to increase in sonication time (Fig. 2d). The PXRD pattern of GN@CSDs shows peak at ($2\theta=26.5^\circ$) which was also observed in control graphite powder (Fig. 2e). AFM image of GN@CSDs (Fig. 2f) confirms the exfoliation process along with adsorption of N@CSDs onto the sheets.

Abstract ID: 129

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Polymeric composites

Keywords: MWCNT, Nafion composite; Ammonia recovery

Enhanced ammonia recovery from wastewater using a MWCT/Nafion composite membrane

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Nitrogen removal in wastewater by conventional treatment methods requires substantial energy, only to release it back to the atmosphere as gaseous nitrogen. In this study, a mixture of Nafion ionomer and Multiwall Carbon Nanotubes (MWCNTs) was incorporated into a Poly(vinylidene fluoride-co-hexafluoropropene; PVDF-HFP) nanofiber matrix to fabricate a Nafion membrane that has high recovery of ammonia nitrogen and increased mechanical strength. Theoretical modelling was conducted to predict the expected performance of the fabricated Nafion membrane under different environments and to reveal the mechanism behind the enhanced recovery of Nafion membranes in the MD process. The resultant Nafion (8%)/MWCNT (2.5%)/PVDF-HFP nanofibrous membrane showed up to three times higher ammonia recovery from an ammonia feed at 300 mg/L concentration compared to the commercial PVDF membrane. Theoretical analysis quantitatively revealed that the Nafion containing membrane can not only suppress the negative effect of the membrane's structural resistance on the ammonia removal efficiency but even enhance the efficiency. The Nafion effect on the ammonia removal efficiency was maximized when the Nafion 6% membrane was employed. This study demonstrated an innovative and realistically applicable MD treatment process that enables resource recovery using low-grade heat and has scaling-up potential for wastewater treatment plants.

Abstract ID: 130**Symposium 2: Functional Composite Materials (FCM)****Poster Presentation**

Topics: Polymeric composites

Keywords: HPLC, Chromatography, Separation, Monolithic stationary phases, Itaconic anhydride

Preparation of novel functionalizable polymeric monoliths for specific capillary liquid chromatographic separations

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New approach to the preparation of porous polymer monoliths possessing functional groups has been developed. It comprising continuous beds forming 3D network structure, which has a functionalizable group enabling post-synthetic modification to immobilize molecules of a desired interaction nature to the monolith, characterized in that these groups are itaconic anhydride units. Monolithic capillary columns for liquid chromatography were prepared by an in-situ polymerization procedure using itaconic anhydride as a monomer and ethylene dimethacrylate as crosslinker. The itaconic anhydride enables post-polymerization modification of the monolithic columns via amidation with a suitable amine for specific separations. The main advantage of monolithic materials is the presence of interconnected channels forming a continuous network structure. The continuous bed monolithic materials are characterized by a bimodal pore structure with a large through-pores provide monoliths with high permeability compared to conventional macroporous materials, and a small micropores leading to more efficient separation and/or purification. The aim of post-polymerization modification is to separate the selectivity of the monolithic media from its morphology. The modification of surface chemistry after polymerization to meet the desired application in a morphologically optimized monolithic media lead to high efficiency and reproducibility. A straight forward method for post-polymerization modification is to include a reactive monomer such as glycidyl methacrylate, N-acryloxysuccinimide, vinyl azlactone or maleic anhydride into the monolithic matrix, which could be modified later to the desired surface chemistry. In this study, the capillary monolithic columns have been prepared using a mixture containing itaconic anhydride and ethylene dimethacrylate in a binary porogenic solvents composed of toluene and 1-dodecanol. The columns were prepared by thermal polymerization in 0.32mm (i.d.) × 150mm fused silica tubing. After polymerization, the columns washed using acetonitrile and then modified using two different amines, octadecyl amine and benzyl amine. Octadecyl amine provides the columns with a hydrophobic C18 group leading to a very good separation of successive alkyl benzene members (toluene, ethyl benzene, propyl benzene and butyl benzene). The other group of columns modified using benzyl amine immobilizes an aromatic benzene ring allowing the separation of various aromatics such as benzene, naphthalene and anthracene. The chromatographic properties were investigated for the two groups of columns. This work open up new aspects representing functionalities within the monolithic stationary phase. The added function groups may bring a variety of properties suitable for various applications such as; positive or negative electric charges, chiral selectors, specific groups, catalytic sites.

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Abstract ID: 131 / Poster: 23

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Ceramic based composites

Keywords: CeO₂, Heterojunction, Sensor

Growth of nickel oxide on CeO₂ nanoparticles obtained in different morphologies applied as gas sensor

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Particles of CeO₂ has shown important role to emerging technological areas of environment and energy (1,2). The mechanisms of reactions are altered in order to favor the preferential growth of the particles, such as time, pH and directing agents causing alteration in the surface defects and consequently changes of their electrical properties (3). The morphological and structural properties of CeO₂ nanoparticles were examined as a function of time and catalytic agent concentration used in the microwave assisted hydrothermal synthesis method. We obtained particles of CeO₂ in different morphologies: beans, rods, and hexagons. Then we obtained, via a wet route, the growth of nickel oxide on the surface of the cerium oxide particles. We discuss the obtaining of the different morphologies and the formation of the heterojunctions through Raman and photoluminescent spectroscopies, X-ray diffraction and transmission electron microscopy, and the electronic properties was evaluated through theoretical calculations by DFT and electrical measurements as function of temperature. This research explores the physicochemical properties of particle growth in different morphologies and tensions of the crystalline lattice existing between the CeO₂ preferential surfaces with Ni₂O₃, forming the heterojunction with respect to the CO gas sensing application.

Abstract ID: 132 / Poster: 39

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Silver nanoparticles, Porphyrin, Photodynamic therapy

A potential mediator for photodynamic therapy based on Silver nanoparticles functionalized with porphyrin

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The development of photodynamic agents (PDT) based on metal nanoparticles loaded with porphyrin derivative has been explored in present investigation. For this purpose, a novel porphyrin derivative 5,10,15,20-Tetrakis(2,4-dihydroxyphenyl) porphyrin (POR) has been synthesized and characterized at molecular scale. The synthesized POR has been loaded on the surface of simply prepared using silver nanoparticles with mercaptosuccinic acid as capping agent (MSA-AgNPs). The formation of newly designed nano composite system (POR-MSA-AgNPs) has been supported by different characterization techniques such as UV–Vis absorption spectroscopy, fluorescence spectroscopy, X-ray photoelectron spectroscopy (XPS) and Field emission scanning electron microscopy (FE-SEM). In order to investigate the capacity of synthesized nano system as efficient photosensitizer in PDT, the efficiency of singlet oxygen generation for POR-MSA-AgNPs and free molecule POR has been successfully examined. The decay in absorbance of 9,10-Dimethylanthracene (DMA), showing an superior efficiency of singlet oxygen production when the POR is incorporated onto the MSA-AgNPs than its free form. Thus, the efficient singlet oxygen production of POR-MSA-AgNPs together with excellent photophysical characteristics and hydrophilic nature opens a new window to explore it as PDT agent along with great potential in bioanalytical applications, drug formulation and biosensing.

Abstract ID: 133

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Rhodamine 6G dye, Chemosensor, Mercury ion

A rhodamine based highly selective and sensitive “off- on” chemosensor for detection of Hg²⁺ metal ion in aqueous media

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A highly selective and sensitive turn-on chemosensor based on rhodamine 6G dye for Hg²⁺, N-(3',6'-bis(ethylamino)-2',7'-dimethyl-3-oxospiro[isoindoline-1,9'-xanthene]-2-yl)-4-fluorobenzamide (SB) has been developed. The synthesized compound was confirmed by using ¹HNMR, ¹³CNMR and LC-MS technique. Studying its fluorogenic behaviors towards various metal ions, prominent fluorescence enhancement was observed for Hg²⁺ over other coexistence metal ions. A prominent fluorescence enhancement was observed in the presence of Hg²⁺, which were escorted by ring opening of a rhodamine Spiro-cyclic structure. The stoichiometric ratio and association constants of the complexes between SB and Hg²⁺ have been measured and calculated. The stoichiometric ratio of the SB-Hg²⁺ complexes was determined to be 1:1 according to a Job's plot experiment. The extreme fluorescent enhancement caused by Hg²⁺ binding in chemosensor SB occurred at a pH range of 6-8.

Abstract ID: 134

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Electrocatalysis

Keywords: mesoporous, materials, overpotential, water oxidation

Iron-Cerium Based Electrocatalyst for Water Oxidation

Jony Saha^{1,2}, Radhakrishnan T P¹

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Iron-Cerium Based Electrocatalyst for Water Oxidation

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Fe based materials despite being cheap and highly abundant received much less attention in water oxidation catalysis. Intrinsic poor electrical conductivity of iron oxides/hydroxides/phosphate leading to slow transfer of electrons with the underlying conductive substrate has been acknowledged to be competent reason. We report a synthesis of mesoporous Ce incorporated FePO₄.FeOOH (FeCePH) films by soft chemical strategy involving CTAB surfactant in view of mutualistic impact of Fe (III) and Ce (III).¹ The materials were characterized by spectroscopic (FT-IR, Raman and X-ray photoelectron spectroscopy) and microscopic (FESEM and TEM) analyses. FeCePH films showed initial improvement in catalytic activity with increasing cerium in the water oxidation at pH=7. Overpotential and Tafel slope decreased from 806 to 690 mV and 104 to 86 mV/dec at 1 mA/cm² current density, respectively attaining minima with Fe:Ce ratio of 1:0.5. The enhancement of catalytic activity with increasing cerium in FeCePH evidenced the coupling of Ce³⁺/Ce⁴⁺ with Fe³⁺/Fe⁴⁺ and regeneration of active catalytic site in FeCePH.

Key Words: mesoporous, materials, overpotential, water oxidation

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Abstract ID: 135

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin Films in Photovoltaic Cells and Energy

Keywords: Atomic Layer Deposition; Solar cells; Review; Thin films

Review of Atomic Layer Deposition of Nanostructured Solar Cells

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This study reviews atomic layer deposition technique with a special interest in solar cells applications. Atomic layer deposition is a vapour phase deposition technique used for producing thin films for several applications. This review focuses on the chemistry of Atomic Layer Deposition of solar cells, merits and demerits of ALD on thin film solar cells. Solar cells have attracted a lot of interest due to their potential for affordable, clean and sustainable energy. Solar cells can be deposited using different deposition techniques but Atomic layer deposition currently attracts attention owing to the merits. ALD has functional merit to bulk materials, great processing flexibility and affordability. The review will examine the merits of ALD and solar cells and areas for future study. It offers affordability, ease of control of film growth, conformal and improvement on the deposition of solar cells. Despite few demerits, ALD is poised to be the deposition technique of choice for modifying interfaces of the film for improved performance.

Abstract ID: 136

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Optical, electrical and magnetic properties of thin films

Keywords: SCAPs; Solar cells; Optoelectronic properties; Thin films

Modeling the Optoelectronic properties of Nanostructured metal oxide Solar Cells

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This paper reported numerical modelling of the optoelectronic properties of nanostructured metal oxides (NiO, Cu₂O and TiO₂) heterojunction solar cells. Modelling of solar cells will speed the advancement of affordable, clean and sustainable thin film solar cells. In this study, solar cells equations were modelled and thereafter SCAPs used to model the nanostructured metal oxides optoelectronic properties. Modelling tools were used to validate the influence of NiO, Cu₂O and TiO₂ material features such as deposition temperature, voltage and defects densities on the performances of the heterojunction solar cells structure. The working points used include a temperature of 350 oC, illumination of 1000W/m² using an AM1.5 lamp, the voltage range of 0 to 1.5 volts. The output gave Voc of 0.1445 V, Jsc of 247.959195E-6 mA/cm² and FF of 37.87 % and Voc 0.7056 and Jsc 28.366911mA/cm² when both contacts were added. This open new frontier for modelling of metal oxide based thin films solar cells especially NiO, TiO₂ and Cu₂O thin films solar cells. This is booster in the quest to develop affordable and sustainable energy by encouraging more research in solar cells technologies in low-income countries

Abstract ID: 137

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Anodes and cathodes Materials

Keywords: Carbon felt, Conductivity, Theoretical Description

Theoretical Description of Carbon Felt Electrical Resistance under Squeezing

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Electro-conductive carbon felt (CF) material composed by bonded together different lengths carbon filaments has porous structure and significant internal surface for ensuring rapid electrochemical reactions. Owing good hydro-permeability and electrical conductivity CF found in numerous electrochemical applications for electrodes design in redox flow batteries, fuel cells, electrochemical desalination apparatus etc.

Felt internal structure is composed by bonded together different lengths carbon filaments interconnected each other resulting good electrical conductivity. Its electro-conductivity is ensured mostly by long bonded carbon fibers located between electrodes and touching at the same time both of electrodes surfaces. Electro-conductivity property of CF is extremely important for the efficient activities of different appliances where CF is used including electrochemical cells for diverse purposes. Hence, this property should be studied deeply and essentially.

Improved electrical conductivity is achieved by a small pressing of CF to the direction of conducting electrodes substrate. Increasing stress on a felt provides supplementary electrical contacts of carbon filaments inside a felt that causing improved electrical conductivity. Moreover, internal interconnects enhance an active surface of a felt electrode boosting redox chemical reactions. However, additional CF pressing diminishes its hydrodynamic permeability and this circumstance should be considered for the optimal design of electrochemical cells.

CF electrical properties experimentally studied is shown in numerous publication, a small portion of which is represented here [1-2]. However, instead of a hydrodynamic permeability CF conductivity is not described by strict analytical models. The use of such models can advance both a design of new electrochemical appliances as a manufacturing of CF having improved structure.

The presented article provides comprehensive results of numerous measurements as well as a theoretical model describing CF electrical conductivity based on a stochastic description of carbon filaments dimensions and locations inside its frame. In addition, the influence of liquids having various electrical permittivity on CF conductivity is analyzed.

Abstract ID: 138

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Bioengineering

Keywords: Depression, MicroRNA, Exosome, Biomarker, Diagnosis, Therapy

MicroRNAs and Exosomes in Depression: Potential Diagnostic Biomarkers

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Depression is known as one of important psychiatric disorders which could be associated with disability among various populations. Diagnostic and statistical manual of mental disorders, 4th edition (DSM-IV) and international statistical classification of diseases and related health problems (ICD-10) could be used as subjective diagnostic schemes for identification of mental disorders such as depression. Utilization of subjective diagnostic schemes are associated with limitations. Hence, it seems that employing of new diagnosis platforms is required. Multiple lines of evidence indicated that measurement of several biomarkers could be useful for detection patients with depression. Among of various types of biomarkers, microRNAs (miRNAs) have been emerged as powerful tools for diagnosis patients with depression. MiRNAs are small non-coding RNAs which act as epigenetic regulators. It has been showed that these molecules have critical roles in pathogenesis of many diseases such as depression. These molecules exert their effects via targeting a variety of cellular and molecular pathways involved in initiation and progression of depression. Hence, miRNAs could be used as diagnostic and therapeutic biomarkers in patients with depression. Besides miRNAs, exosomes as nano- carriers could have been emerged as diagnostic biomarkers in several diseases such as depression. These vesicles are able to carry several cargos such as DNAs, proteins, mRNAs, and miRNAs to recipient cells. Here, we summarized several miRNAs involved in pathogenesis and response to treatment of depression which could be used as diagnostic biomarkers. Moreover, we highlighted exosomes as new diagnostic biomarkers for patients with depression.

Abstract ID: 139**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Piezotronics for smart systems

Keywords: PVDF-HFP/TiO₂ nanocomposite, core-shell structure, Energy Storage

Significantly Enhanced Breakdown Field for Core-shell Structured Poly(vinylidene fluoride-hexafluoropropylene)/TiO₂ Nanocomposites for Ultra-high Energy Density Capacitor Applications

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Organic/inorganic nanocomposite materials have been extensively studied for high energy density capacitor applications due to their relatively large dielectric constant. However, most of these nanocomposite materials suffer from a very low breakdown field. In this investigation, poly(methyl methacrylate) (PMMA) grafted titanium dioxide (TiO₂) (TiO₂-g-PMMA) was synthesized through a seeded emulsion polymerization method. Then, the hybrid nanoparticles were incorporated into a poly(vinylidene fluoride- hexafluoropropylene) (PVDF-HFP) film using solution casting to form a PVDF-HFP/TiO₂-g-PMMA nanocomposite. After the characterization, it was revealed that the TiO₂ nanoparticles were perfectly coated with PMMA layer. Further, the dielectric measurement results showed that the permittivity nanocomposite was enhanced by 13.9% as compared with the pristine PVDF-HFP film. The polarization loop data of the nanocomposite indicated that the highest breakdown field and energy density of the PVDF-HFP film with 1 vol.% TiO₂-g-PMMA reached 560 MV/m and 14.2 J/cm³, respectively. The breakdown field of the nanocomposite with grafting is doubled as compared with the nanocomposite without grafting. Further, as compared the pristine PVDF-HFP at same electric field, the energy density of the PVDF-HFP/TiO₂-g-PMMA nanocomposite (1 vol.%) is increased by 14.4% (from 12.4 to 14.2 J/cm³). The nanocomposite film also showed an improved charge-discharge energy efficiency of 47% under 500 MV/m electric field, which was much higher than pristine PVDF based polymer. The PVDF-HFP/TiO₂-g-PMMA nanocomposite shows a great promise for future high energy density capacitor applications.

Thursday, 22/Aug/2019 3:27pm - 3:39pm

Abstract ID: 140 / FESC-2: 8

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Hybrid cells for energy harvesting

Keywords: Poly-yenes; Poly(metalla-yenes); Opto-electronics.

Poly-yenes and Poly(metalla-yenes) for Opto-Electronic (O-E) Applications

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Poly-yenes and poly(metalla-yenes) are fascinating new materials for applications in diverse opto-electronic (O-E) devices such as light-emitting diodes, solar cells and non-linear optics. [1-3] Three types of metalla di-, oligo- and poly-yne materials are extensively investigated in our

laboratories. The first series consists of phenothiazine (PTZ) based organic co-polyynes incorporating a wide variety of conjugated spacers. The second series consists of Pt(II)-Re(I) based hetero-bimetallic poly-ynes. The incorporation of a second metal ion such as Re(I) have been linked with the induction of D-A interaction, leading to reduction in the band gap of the material, an important factor in the determination of O-E properties. The third series is comprised of metal organic framework (MOF) materials, self-assembled aryl ethynylpyridine and Cu(I) halide complexes.[4] The design, synthesis, electro-chemistry and the effect of different aromatic spacers on the structural, electronic and optical properties will be presented. In addition, photo-voltaic potential of the materials will be presented with structural analysis of the model compounds.

Key Words: Poly-ynes; Poly(metalla-ynes); Opto-electronics.

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Abstract ID: 141

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biomaterials for soft tissue applications

Keywords: Hydrogel, Cartilage, Dissipation, Tissue engineering

Enhanced mechanical and mechanobiological properties of hydrogels by controlling their dissipation sources

Naser Nasrollahzadeh, Peyman Karami, Dominique Pioletti

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Dissipation plays an essential role in the mechanical behavior of materials under cyclic loading. In particular for soft materials, insufficient dissipative capacity is known as the main reason for the low toughness and inability to resist defect growth in hydrogels. In parallel, a new paradigm on the role of dissipative phenomena in the field of soft tissues and biomaterials recently emerges through observations of relation between dissipation and mechanobiology. Dissipation may therefore be related to two different but complementary objectives in the development of hydrogels: increase their fatigue resistant properties and induce new mechanobiological features. By considering an hybrid crosslinking strategy presenting weak physical reversible bonds and strong covalent bonds in a single network pHEMA based hydrogels in parallel with a dual porosity design encompassing nano meshes and meso pores, we were able to modulate the importance of the dissipation sources originating either from flow-independent or flow-dependent processes. Herein, we report that by an optimized combination of dissipation sources, fatigue resistant hydrogels can be developed presenting similar range of compressive stiffness, dissipation, and water content compared to cartilage. This optimized combination of dissipation sources which preserved the mechanical hysteresis during cyclic compression, also positively impacted the mechanobiological feature of the hydrogel as chondrogenesis was favored in these cell seeded hydrogels. The careful consideration of dissipation sources in the development of hydrogels opens therefore new possibilities for fine-tuning their mechanical behavior in a biological environment.

Key Words: Hydrogel, Cartilage, Dissipation, Tissue engineering

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Wednesday, 21/Aug/2019 5:12pm - 5:24pm

Abstract ID: 142 / FCM: 7

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Ceramic based composites

Keywords: Graphene, Polymer Derived Ceramic, Composites

Polymer Derived Ceramic Composites with Graphene

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Polymer derived ceramics (PDCs) include a class of ceramics (e.g. SiC, SiCO, SiCN, BCN, BN, Si₃N₄, and etc.) synthesized by a thermal decomposition of polymeric precursors. PDCs have unique nanostructures that grant various attractive properties such as low density (~2g/cm³), excellent high-temperature thermo-mechanical properties (up to 2000oC), high piezoresistivity and chemical/thermal stability. These unique properties lead to various potential applications including electromagnetic interference shielding (EMI), energy storage devices, catalysts, thermoelectrics and etc. Fully dense bulk SiCO ceramics were fabricated with embedded graphene aerogels (GAs) and graphene oxide (GO). To produce green body composites, the polymer precursors (i.e. oligosilazane and polysiloxane) were filled in GA and GO porous structures followed by crosslinking. These green body composites were cut into difference shapes and pyrolyzed into ceramic composites. The graphene network plays a dual role in both systems, as a reinforcing frame maintaining the ceramic composite's mechanical properties and as a conductive filler to increase electrical conductivity. 1 % embedded GO increased the electrical conductivity of PDC by more than eight orders of magnitude.

Abstract ID: 143

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Carbon Nanomaterials

Keywords: Surfactant Arrangements, Photoexcitation, Polarization, Dipole Moment Transitions, Zeta Potential, Protonation

Selective Protonation of Sodium Cholate for Reversible Blue-Shift Absorption Spectra of Single-Chirality Single-Walled Carbon Nanotube in Solution

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In contradiction to the long-standing optical depletion of single-walled carbon nanotubes (SWCNT) by acid doping, this work reports the blue-shifted and optical density-increased S₁₁ (the first van Hove singularity transition) peak absorption spectra of single-chirality (6,5) SWCNT dispersed in specific surfactant compositions such as 1% SDS (sodium dodecyl sulfate) /1% SC (sodium cholate) and 2% SDS/0.5% SC, which were caused by addition of acid. These anomalous optical changes can be reversed by adding base, and are discussed on basis of surfactant arrangements on SWCNT sidewalls, which arose from the selective protonation of free SC to shift the thermodynamic equilibrium of SC adsorbed SWCNT to the desorption of SC from SWCNT surface. The spectroscopic interpretation obeys the dipole moment transition related energy level variation and oscillator strength change.

Abstract ID: 144

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Composite structural materials

Keywords: Polyamide 6, Organoclay, Montmorillonite, Nanocomposite, exfoliation.

Effect of Organic Modifier Loading on Particle Dispersion of Nanocomposites Based on Polyamide 6 and Natural Montmorillonite

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Nanostructured polymers have attracted much attention in material sciences because of their unique properties and their applications in nanomaterials and nanodevices. In this study; natural sodium montmorillonite (NaMMT), Cloisite Na⁺ and two organophilic montmorillonites (OMMTs), Cloisites 20A and 15A (have the same organic modifier with a loading of 90 and 125 meq/100g clay, respectively) were used. Polyamide 6 (PA 6) / NaMMT nanocomposites containing 1, 3, 5, and 10 wt% Cloisite Na⁺ and PA 6 / OMMT nanocomposites containing 5 and 10 wt% Cloisites 20A and 15A were prepared via melt compounding using a twin screw extruder. Thermal stabilities of the obtained composites were characterized by TGA which confirmed moderate thermal stability enhancement of PA 6 after adding 5 wt% of filler in the sequence: Cloisite Na⁺ < Cloisite 20A < Cloisite 15A, whereas thermal stabilization was less efficient at 10 wt%. The interaction between PA 6 chains and silicate layers was studied by FTIR spectroscopy which confirmed strong interactions between nanometric silicate layers and nylon 6 segments. The electrical conductivity (σ) which describes the ionic mobility of the systems showed that σ of PA 6 was greatly enhanced on increasing the organic modifier loading at filler content of 5 wt%, especially at higher temperatures in the sequence: Cloisite Na⁺ < Cloisite 20A < Cloisite 15A. The obtained values are situated between the two extremities of those of semiconductors (10^{-10} – $10^{-2} \Omega^{-1} \text{cm}^{-1}$) of which σ of PA 6 / 5 wt% Cloisite 15A nanocomposite was increased by ten orders of magnitude higher than that of pristine PA 6. These values were then decreased with further increasing the filler content to 10 wt%. This may be attributed to the formation of some nanoparticle agglomerates due to more intense interfacial interactions between nanoparticles rather than between nanoparticle and PA 6 matrix upon further increasing the content of the filler, which may cause some steric hindrance that partially contributes to decreasing the electrical charge mobility. The activation energy (E_a) obtained from the dependency of σ on temperature using Arrhenius equation was the lowest for the nanocomposite containing 5 wt% Cloisite 15A. Strong interfacial interactions between silicate layers and PA 6 chains effectively enhanced mechanical properties of PA 6 on using 5 wt% of clay in the sequence: Cloisite Na⁺ < Cloisite 20A < Cloisite 15A, whereas further increasing to 10 wt% resulted in a deterioration in these properties. PA 6 crystallization behavior and the dispersed behavior of clay in PA 6 matrix were evaluated by XRD, TEM, SEM, and DSC analyses which revealed that only a small amount of clay accelerated the degree of crystallinity and crystallite sizes and revealed exfoliated structures in PA 6/5 wt% OMMT nanocomposites.

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Abstract ID: 145 / Poster: 32

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Dielectric, Ferroelectric and Piezoelectric materials

Keywords: Metamaterials, negative dielectric constant, perovskites, Correlated Barrier Hopping conductivity.

Negative Dielectric Constant Property of $\text{EuSr}_2\text{CaCu}_2\text{O}_{6.5}$ Ceramic

Ibrahim Incedal, Yaşar Karabul, Mehmet Kılıç, Orhan İçelli, Zeynep Güven Ozdemir

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Materials with negative permeability and permittivity have attracted great attention due to their exotic electromagnetic properties. Especially, synthesis of novel negative dielectric constant (NDC) materials is the fundamental step for developing metamaterials or artificial negative index materials. From this point of view, to produce a novel NDC material, $\text{EuSr}_2\text{CaCu}_2\text{O}_{6.5}$ ceramic was synthesized by conventional solid-state reaction method. The surface morphology of the sample was determined by Scanning Electron Microscope (SEM). The real and imaginary components of the complex impedance and dielectric function of the sample were measured between 1 Hz and 40 MHz frequencies at different spot temperatures varying from 293K to 433K. The NDC property was observed above 353 K at the low-frequency region. The temperature dependence of the real part of the complex impedance versus frequency curves of the ceramic implied the semi-conducting nature of the sample. The imaginary component of complex impedance also indicated temperature dependent relaxation process in the material. It was revealed that while the low-frequency conductivity mechanism of the sample is independent of frequency, the sample exhibits Correlated Barrier Hopping mechanism for the charge transport at high frequency. Ultimately, it can be concluded that the $\text{EuSr}_2\text{CaCu}_2\text{O}_{6.5}$ has a promising potential for metamaterial coating applications.

Abstract ID: 146

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Nanocomposites

Keywords: Polymer/nano particle composite, Impedance Spectroscopy, Ac conductivity.

Synthesis, Structural and Dielectric Characterization of Polyindole-Silver Nano Composites

Sermin İlayda Ozkan, Seda Erdönmez, Mehmet Kılıç, Yaşar Karabul, Orhan İçelli, Zeynep Güven Ozdemir

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Polyindole (PIn), which is a conductive polymer containing benzene ring linked with the pyrrolic ring [1], has good thermal stability, high redox activity, and slow degradation rate [2,3]. Due to its remarkable properties, PIn and PIn based nano composites have been utilized in various applications such as battery [4], sensor [5], drug delivery [6]. Since depending upon the synthesis techniques and the nature of the filler, the properties of the composites can be changed to reach desirable properties for various applications. In this respect, the PIn/Ag nano composites were synthesized for modifying the PIn conductivity for potential technological applications. PIn and nano silver particles were synthesized by chemical oxidative polymerization and hydrothermal methods, respectively. PIn was doped with different wt. percentages of nano Ag particles. The structural morphology of the samples was investigated by Scanning Electron Microscopy (SEM). The Fourier Transform Infrared (FTIR) Spectroscopy was used to determine the chemical structure of the samples. The thermal stability of the samples was investigated by Thermogravimetric Analysis (TGA). The complex impedance measurements were performed in the frequency interval between 10 Hz and 40 MHz. The frequency dependences of the real and imaginary parts of the complex impedance and complex dielectric functions were investigated in details. The effect of Ag nano particle loading on PIn's ac conductivity of was also discussed.

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Wednesday, 21/Aug/2019 6:00pm - 6:12pm

Abstract ID: 147 / FCM: 11

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Polymeric composites

Keywords: Radiation Shielding, Epoxy Resin, Nano Composite, Monte Carlo Simulation

Epoxy/WO₃ Nano Composites as an Eco-Friendly Gamma Ray Shielding Materials

Isa Emin Ongun¹, Yaşar Karabul¹, Mustafa Çağlar², Mehmet Kılıç¹, Zeynep Güven Ozdemir¹, Orhan İçelli¹

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A wide variety of radiation shielding materials are utilized to protect both human's health and nearby electronic instruments from the harmful effects of ionizing radiation sources. Among radiation shielding materials, concrete and lead are the most utilized materials. Although concrete and lead are good radiation shielding materials, they have several disadvantages such high weight, toxicity, non-transparency. Therefore, non-toxic, lead-free, low weight and transparent polymer composites that are reinforced with high Z elements have a promising potential in radiation shielding industry. From this point of view, epoxy resin/WO₃ nano composites were prepared with different WO₃ nano particle weights percentages varying from 5 to 20. The WO₃ nano particles were synthesized by hydrothermal method. The effect of gamma radiation on the samples' thermal properties was investigated by Differential Scanning Calorimetry (DSC) analysis. The distribution of WO₃ nano particles in the epoxy matrix was also viewed by Scanning Electron Microscope (SEM). The influence of WO₃ nano particle loading on the gamma-ray shielding performance of the samples was determined experimentally by utilizing two different energy peaks of Ba-133 point source. The mass attenuation coefficient, half layer value, mean free path and effective atomic number Z_{eff} of the samples have been measured for 81 keV and 356 keV energies. The same parameters were also determined by Monte Carlo N-Particle (MCNP) simulation. Since there is a good agreement between experimental and simulation results, Monte Carlo N-Particle (MCNP) simulation was carried out to obtain theoretical prediction of the gamma ray shielding parameters of the same samples for gamma rays with different photon energies such as 59.5 keV, 80.9 keV, 140.5 keV, 356.5 keV, 661.6 keV, 1173.2 keV, and 1332.5 keV.

Abstract ID: 149

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Surface treatment and Interface control

Keywords: Calcium Sulphide, Scalar wave Thin Film, Dielectric Perturbation, Green's Function, Dyson's Equation, Born approximation, Wave Propagation Solid State and Optical Properties

Theoretical Approach to Study the Solid State and Optical Characteristics of calcium Sulphide[CaS] Thin Film.

Emmanuel Ifeanyi Ugwu

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Calcium sulphide thin film has been studied in this work using theoretical approach in which a scalar wave is propagated through the material thin film deposited on a glass substrate with the assumption that the dielectric medium has homogenous reference dielectric constant term, and a perturbed dielectric function, representing the deposited thin film medium on surface of the glass substrate is presented in this work. These two terms, constituted arbitrary complex dielectric terms that describes dielectric perturbation imposed by the medium of for the system. This is substituted into a defined scalar wave equation in which the appropriate Green's Function in conjunction Dyson's equation was defined on it to reduce it to Volterra equation of second type with the kernel is solved using series solution technique in conjunction with Born approximation method in order to obtain a model equation of wave propagating through the thin film. This was used in computing the propagated field, for different input regions of field wavelength such as ultraviolet, visible and infrared region respectively during which the influence of the dielectric constants of the thin film on the propagating field were considered. The results obtained from the computed field were used in turn to compute the band gaps, solid state and optical properties of the thin film such as reflectance, Transmittance and absorbance.

Keywords; Calcium Sulphide, Scalar wave Thin Film, Dielectric Perturbation, Green's Function, Dyson's Equation, Born approximation, Wave Propagation Solid State and Optical Properties

Abstract ID: 150

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalytic transformation of CO₂

Keywords: Carbon, Topological Structure, CO₂ Reduction, Electrocatalysis

Engineering Carbon Topological Nanostructure for Electrocatalysis of Carbon Dioxide Reduction

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Electrocatalytic reduction of CO₂ into value added chemicals or fuels is a promising technique towards a carbon-neutral chemical process. The electrochemical reduction of CO₂ is a complicated process involving multiple protons coupled electron transfer, theoretically resulting in a variety of products (e.g. CO, HCOOH, CH₄, C₂H₄ and C₂H₅OH). Therefore, the major challenge in CO₂ reduction lies in the manipulation of the selectivity towards a specific product as demanded. However, the study on CO₂ reduction has not substantially advanced primarily because of the lack of fundamental understanding of the reaction mechanism and the challenge of discovering efficient and robust catalysts for the various multi-electron transfer processes. Researchers have screened a wide range of metal-based materials for electrochemical reduction of CO₂, and found only copper-based metals exhibit selectivity towards formation of multi-carbon hydrocarbons and oxygenates at fairly high efficiencies while most others favor production of carbon monoxide or formate. Beyond Cu, we have recently shown metal free N-doped graphene quantum dots (NGQDs) can yield C_{≥2} products. When enriching the N-doping at the edge of carbon nanostructures, the NGQDs exhibit exceptional activity towards formation of C₂H₄ and C₂H₅OH with a combined Faradaic efficiency of 40% and a partial current density of 100 mA cm⁻² at a low overpotential. Here we will present how the carbon topological nanostructure can be further engineered to tune the catalytic activity and selectivity towards CO₂ reduction with an emphasis on the production of C_{≥2} products. We will discuss the key structural and electronic factors that governs the performance of carbon-based catalysts. This study provides in-depth insights for developing high-performance carbon-based catalysts for electrochemical reduction of CO₂.

Abstract ID: 151

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: Self-healing Material, Thermal Barrier Coating, Alloy, Composite

A Novel Functional Self-Healing Metallic Composite

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A novel functional self-repaired high temperature iron based coating alloy was developed. The alloy was tested for heat and oxidation resistance on three substrates, such as two mono-crystals Nb and Mo and polycrystalline low alloyed Cr samples. The composition of the alloy is Fe-45%Cr-4%Al-1%Ni-0.3%La. The test specimens were prepared using an electron-beam vacuum evaporation technique followed by a thermal-chemical treatment at 1200OC. The compositions were investigated using the SEM, WDS, AES and LM techniques. The results of the tests showed that the newly developed coating layer at high operation temperatures has an ability to repair the cracks developed as a result of both mechanical and thermal damages. Due to the high adhesion with the metallic substrates, this coating composition also has an ability to protect against high temperatures, corrosion and a wear.

Abstract ID: 152

Symposium 2: Functional Composite Materials (FCM)

Invited Talk

Topics: Bio-inspired design of composites

Keywords: Smart materials, Photonic crystals, shape-transformation

Bioinspired composite material-based actuators and their applications

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Bioinspired composite materials are originated from the inspiration of nature, such as chameleon and Venus flytraps. Due to their intriguing properties, these materials have been wisely explored in various research fields like sensors, actuators, etc. Here, we would like to present our recent progress on chameleon-inspired structural color materials firstly, including bio-inspired fabrications and sensing applications. Then, the Venus flytraps-like actuators, which can change their shapes accordingly after triggered with specific solvent, near-infrared light and temperature, are followingly introduced. Based on the rapid progress in this field, we believe bioinspired polymers will find great potential applications in wearable and implantable devices.

Abstract ID: 153**Symposium 6: Functional Thin Films (FTF)****Oral Presentation**

Topics: Thin Films in Photovoltaic Cells and Energy

Keywords: ZnS, annealing, bandgap, Urbach energy, dielectric constants

Taming the optical and morphological properties of chemically deposited Zinc Sulphide thin films for use in sustainable energy devices**ROBERT BEN JOSHUA**

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The chemical bath deposition technique was used to grow thin films of zinc sulphide (ZnS). The films were grown at different concentrations (0.1 M – 0.4 M) and other deposition variables were kept constant. The films were subjected to post-deposition heat treatments with annealing temperatures in the range 373 K to 573 K. The effect of the different precursor concentrations and annealing treatments on the films were investigated with emphasis on the morphology, and optical properties such as transmittance, absorbance, reflectance, optical absorption coefficient, energy bandgap, refractive index, and the dielectric constants. The electrical resistivities of the layers were also deduced from the optical measurements. The results indicate that the different annealing temperatures and precursor concentrations influenced the morphology, film thicknesses, optical and electrical properties significantly. In particular, the film thickness were found to vary with post-deposition heat treatments in one direction while the film thickness of the different precursor concentration (Zn^{2+}) varied in the reverse direction. The energy bandgap obtained were direct, and decreased for the annealed layers from 3.80 eV, 3.76 eV, 3.74 eV, and 3.65 eV respectively for as-grown, annealed at 373 K, 473 K and 573 K respectively. However the increase in precursor concentration increased the energy bandgap from 3.72 eV, 3.80 eV, and 3.85 eV for precursor concentration (Zn^{2+}) corresponding to 0.1 M, 0.2 M, and 0.3 M respectively. The annealing treatments induced a red-shift (longer wavelengths) in the fundamental absorption edge while the increase in the concentration of the Zn^{2+} ions exhibited a blue shift (shorter wavelengths) in the fundamental absorption edge thus resulting to higher photon energies. The results also show that a linear relationship exists between the energy bandgap and the Urbach energy. The Urbach energy decreased from 3.40 eV to 3.08 eV for the annealed layers and increased from 3.30 eV to 3.48 eV for increasing precursor concentrations. The dielectric constants of the annealed layers was in the range 2.25-5.75 while the increase in the Zn^{2+} concentration resulted in values of dielectric constants between 2.20-6.0. The values of the energy bandgap and the dielectric constants strongly suggest the use of the films in various solar architecture and in different sustainable energy devices including window layers in thin film hetero-junction solar cells.

Wednesday, 21/Aug/2019 7:15pm - 7:27pm

Abstract ID: 154 / FC: 17

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: New concepts in catalyst design and preparation

Keywords: Organometallics, Carbon-Based Materials, Electrocatalyst

Coordination chemistry of organometallic molecules with carbon-based materials and their catalytic applications

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Organometallic compounds have been a center of molecular catalysts with preeminent catalytic activity and selectivity in a wide range of chemical transformations. The generation of molecularly dispersed active species on the surface of carbon-based network enables to utilize advantages of molecular catalysts as well as to extremely expose active species without aggregation at the surface. In this presentation, I will discuss my recent research activities on this concept. Novel hybrids were generated by the reaction of Co-containing organometallic molecules and carbon-based materials such as chemically modified graphenes, carbon nanotubes, and carbon nitrides. Various chemical analyses confirmed the preservation of the core Co structure in the complex as well as coordination of N-containing species of the carbon-based materials to the Co. The hybrids showed excellent electrocatalytic activity for the oxygen reduction reaction (ORR) in alkaline media, which is comparable to other Co-based efficient catalysts and a commercial Pt/C. Both structural understanding and electrochemical measurements with control samples found that the Co-based species were well-dispersed as molecular entity on the surface and served as highly efficient active species for ORR. This approach to catalyst preparation in conjunction with an understanding of its chemical structure and coordination nature is a promising model for the design of advanced catalysts for other important reactions.

Abstract ID: 155

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nanomaterials for Energy and Environmental Applications

Keywords: molybdenum oxide, hydrogen evolution, morphology

Molybdenum Oxide Nanostructures for energy applications

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MoO₂ nanomaterials are gaining significance due to their high catalytic activity for electrochemical hydrogen evolution, supercapacitor electrodes and also as surface enhanced Raman scattering substrates. We have synthesized MoO₂ nanostructures in powder form as well as a film on fluorine doped tin oxide (FTO) glass through hydrothermal process involving citric acid (CA) as the surfactant. The film on FTO consists of disc-shaped nanoparticles whereas powder form contains microspheres formed by such discs. A systematic growth study performed by varying synthesis conditions indicate that a slight variation in temperature and pH lead to the formation of different polymorphs and diverse morphology of MoO₂ ranging from disc, flower and hexagonal to square rods etc. Metallic nature of the film was revealed from I-V measurements. IR and NMR studies revealed the role of CA as a reducing agent and as a structure directing agent. The electrochemical studies reveal that MoO₂ nanostructures are excellent candidates for hydrogen evolution reaction (HER). HER catalytic activity including the onset potential, current density, and Tafel slope of MoO₂ nanostructures are improved effectively by hydrogen annealing and MoO₂/FTO displays low onset overpotential of 70 mV with a Tafel slope of 84.1 mV dec⁻¹ whereas powder form exhibits onset overpotential of 46 mV with Tafel slope of 71.6 mV dec⁻¹. The large active surface area, exposure of fringe facets of (110) and lesser electrochemical charge transfer resistance offered by the hydrogen annealed MoO₂ play a major role in the enhanced HER activity. Recently, we have been able to achieve rapid synthesis of porous MoO₂ for energy storage application as well.

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Abstract ID: 156

Symposium 2: Functional Composite Materials (FCM)

Invited Talk

Topics: Polymeric composites

Keywords: Hydrogels, hollow tubular networks, water fluidics

Hollow hydrogel networks for temperature-controlled water fluidics

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Hydrogel tubes (HTs) are essential components in nerve guidance channels, uniaxial sustained molecular release and cell adhesion. Fabrication of multiply branched hollow hydrogel tubes is still a challenge, and an effective method is not available yet. We herein develop a cost-effective, facile method for synthesis of multiply branched hollow HTs by direct conversion of single-layer alginate films to HTs in aqueous solution. The process does not require special conditions, and HTs of arbitrary morphology and connectivity can be prepared in a couple of minutes. The method provides access to branched HTs and HT nets and grids of arbitrary shape and topology without the necessity to use templates or molds. The wall of branched HTs can be functionalized to satisfy various application requirements, which are demonstrated by controlled fluidics at high and low temperatures, respectively. The hollow branched HTs can be used as templates for preparation of other tubular networks with improved mechanical properties. Functionalized HTs can be designed into a soft device for temperature-controlled water fluidic.

Thursday, 22/Aug/2019 2:00pm - 2:15pm

Abstract ID: 157 / FCM-4: 1

Symposium 2: Functional Composite Materials (FCM)

Keynote

Topics: Bio-inspired design of composites

Keywords: Bioinspired, Wettability, Nano, Water collection, Water repellency

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

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Biological surfaces in nature (e.g., spider silk, cactus spine, beetle back, butterfly wing, lotus leaf, etc.) have inspired us to design the functional materials and surfaces [1-2]. Inspired by the structures of spider silk for directional water collecting ability, a series of bioinspired gradient fibers has been designed by integrating fabrication methods and technologies, e.g., dip-coating, Rayleigh instability break-droplets, electrospinning, and wet-assembly, etc., thus roughness and curvature, gradient spindle-knots, star-shape wettability pattern, etc. for droplet transport and harvesting. Inspired by cactus spines, the conical spines with periodic roughness or micro- and nanostructures can achieve the high-efficiency condensed-droplet transport. Some dynamic gradient surfaces are also designed, e.g., 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. The bioinspired gradient surfaces can be further designed to exhibit robust transport and controlling of droplets. These bioinspired gradient surfaces would be promising applications into anti-icing, liquid transport, anti-fogging/self-cleaning, water harvesting, etc.[1-5]

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Abstract ID: 158

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Bio-inspired design of composites

Keywords: biomimetics, smart coatings, nanocomposites, mechanical properties, self-healing

An Epidermis-like Hierarchical Smart Coating with a Hardness of Tooth Enamel

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We overcome the fundamental dilemma in achieving hard materials with self-healing capability by integrating an epidermis-like hierarchical stratified structure with attractive mechanical and barrier properties of graphene oxide and show that such biomimetic design enables a smart hierarchical coating system with a synergetic healing effect and a record-high stiffness (31.4 ± 1.8 GPa)/hardness (2.27 ± 0.09 GPa) among all self-healable polymeric films even comparable to that of tooth enamel. A quasi-linear layer-by-layer (LBL) film with constituent graphene oxide is deposited on top of an exponential LBL counterpart as a protective hard layer, forming a hierarchical stratified assembly mimicking the structure of epidermis. The hybrid multilayers can achieve a complete restoration after scratching thanks to the mutual benefit: The soft underneath cushion can provide additional polymers to assist the recovery of the outer hard layer, which in turn can be a sealing barrier promoting the self-healing of the soft layer during stimulated polymer diffusion. The presenting hybridization mode of LBL assembly represents a promising tool for integrating seemingly contradictory properties in artificial materials with potential performances surpassing those in nature.

Abstract ID: 160

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Applications of low dimensional, nano and 2D materials

Keywords: Nano, Doping, Film, Composite, Humidity sensing

Controlling of the microstructure to improve humidity sensing behaviors of titania based nanofilms by RE-doping

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Monitoring and auto-controlling of the local humidity environment are important in the fields of industry, agriculture, military and household. Sensors are developed towards miniaturization, integration, intelligence and high reliability due to stringent serving conditions. Therefore, sensing material, as an essential element of sensors, should be improved with high sensitivity and reliability so as to meet the increasing requirements. In the present work, a sol-gel technique and subsequent annealing were used to prepare the rare earth-doped TiO₂ and TiO₂-SnO₂ nanofilms on glass and alumina ceramic substrates on which a comblike Cu electrode was pre-precipitated. Measurements of the XRD, SEM and HRTEM were adopted to examine the microstructure and a self-assembled device was applied to detect their humidity sensing behaviors. Experimental results show that the irregular anatase crystals with a size of less than 10 μm presented in the titania amorphous dried at 100 °C for 24 h. The RE-doped TiO₂-SnO₂ nanofilms are composed of the TiO₂, SnO₂ and CeO₂/La₂O₃ nanocrystals. The pre-precipitated SnO₂ crystals act as a coherent or semi-coherent surface ({110} planes) to improve the transformation of rutile by the attached growth; the CeO₂ fine particles with a size of 2.5 nm precipitated around them to resist their growth. 0.5 wt% of Ce₂O₃ or Ce₂O₃ doped TiO₂-20 wt% SnO₂ films sintered at 500 °C had the best humidity sensing properties, the impedance decreasing from 109 to below 104 Ω in the humidity range of 15-95 RH%. Moreover, the ceramic substrate had better support to response humidity than the glass substrate; the Ce³⁺-doping has better humidity sensing properties than La³⁺-doping.

Abstract ID: 161

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Exfoliation and unzipping 2D materials

Keywords: Defect-rich, Cryo-pretreatment, MoS₂ nanosheets, Electrocatalyst, Hydrogen evolution reaction

Synthesis of water-soluble defect-rich MoS₂ ultrathin nanosheets for enhanced hydrogen evolution reaction

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Electrocatalytic hydrogen evolution reaction (HER) is accepted as a sustainable method to generate hydrogen from water splitting.^{1,2} Exploring earth-abundant, low-cost alternative catalysts with high HER activity is highly demanded. Herein, we synthesize the water-soluble defect-rich MoS₂ ultrathin nanosheets (d-MoS₂ NS) through a facile cryo-mediated liquid phase exfoliation method with the assistance of NaBH₄. The NaBH₄ was firstly used in liquid phase exfoliation. The cryo-pretreatment in liquid nitrogen facilitates the efficiency of liquid phase exfoliation by weakened the interlayer Van der Waals force between MoS₂ layers. NaBH₄ in the solvent continuously releases H₂ gas that can not only enter the MoS₂ interlayer to cause abundant edge sites on the basal plane of MoS₂ nanosheets but alter the surface property from hydrophobic to hydrophilic nature. The as-prepared d-MoS₂ NS shows enhanced electrocatalytic hydrogen evolution reaction (HER) performance than that of MoS₂ NS due to the hydrophilia and abundant active edge sites. The formation process of the d-MoS₂ NS with exposed edge sites is illustrated by investigating the influence of exfoliation time on the morphological structure of MoS₂ nanosheets. As an electrocatalyst for HER, the d-MoS₂ NS exhibits small overpotential of 71.5 mV at a current density of -10 mA cm⁻² with a low Tafel slope of 58.8 mV dec⁻¹.

Abstract ID: 162**Symposium 2: Functional Composite Materials (FCM)****Poster Presentation**

Topics: Carbon and metal oxide based composite materials

Keywords: Graphene, Prussian Blue, Magnetite, Cesium adsorption

Selective removal of radioactive cesium in water using magnetic Prussian blue graphene based nanomaterial**Humaira Shahzad**

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The radioactive Cesium (half-life of 30 years) is hazardous as it has high solubility, mobility in environment and also emits strong gamma rays and beta particles which exert toxic effects. Many adsorbent materials studied for Cs removal from contaminated water but for large-scale these are either very costly or hard to prepare. Prussian Blue (PB) has shown strong affinity towards Cs, while separation of its ultra-fine powder from water after Cs adsorption makes it problematic. Nevertheless, separation of adsorbent from waste water by magnet after adsorption process is an appropriate method to recover adsorbent from wastewater but the magnetic nanomaterials are easily aggregated due to magnetism and large active surface. Moreover, graphene oxide (GO) has proven to be non-toxic and biodegradable among all carbon nanomaterials and could be produced in bulk quantities. It has high surface area which makes it suitable adsorbent material for environmental applications. However, it is difficult to separate it from aqueous solution as GO forms a stable colloidal suspension in water after Cs adsorption. In order to overcome this problem the current paper provides an ideal solution i.e. fabrication of self-assembled graphene with decorated magnetite PB nanoparticles. The combination of self-assembled nano graphene sheets with large open pores, high specific surface area and magnetic PB nanoparticles might yield enhanced performance.

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Wednesday, 21/Aug/2019 6:39pm - 6:51pm

Abstract ID: 163 / FC: 14

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Photocatalysis

Keywords: Earth-Abundant Catalysts, Hydrogen Production, Photothermal Effect, Photocatalysis

Sonohydrothermal synthesis of noble metal-free Ti@TiO₂ core-shell nanoparticles with advanced photothermal catalytic activity

Sergey Nikitenko, Tony Chave, Xavier Le Goff

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We report synthesis and photocatalytic activity of noble metal-free Ti@TiO₂ core-shell nanoparticles (NPs). Stable to oxidation Ti@TiO₂ NPs have been obtained using innovative sonohydrothermal (SHT) technique consisted of the simultaneous action of ultrasound ($f = 20$ kHz, $P_{ac} = 10$ W) and hydrothermal treatment (200°C, 14 bar) on air-passivated titanium metal NPs (US Research Nanomaterials Inc.) in pure water. HR STEM and Ti, O EDS mapping of initial air-passivated Ti NPs shown reveal the presence of amorphous oxidized shell (appr. 2 nm) at the surface of quasi-spherical Ti NPs with a diameter in the range of 20-80 nm. SHT treatment leads to formation of nanocrystalline shell composed of 5-15 nm anatase crystals. Powder XRD confirmed formation of anatase with a small admixture of rutile. UV/vis/NIR spectrum of Ti@TiO₂ NPs exhibits an absorption band at 308 nm that is due to the bandgap transition of pristine defect-free anatase bandgap energy (3.25 eV). However, in contrast to pristine anatase, Ti@TiO₂ NPs show an extended photo-response from the UV to the NIR light region due to the light absorption by a nonplasmonic Ti core via interband transitions that makes more efficient use of the solar spectrum. It was found that Ti@TiO₂ NPs exhibit much higher photocatalytic activity in H₂ production from aqueous solutions of glycerol (40 % vol.) under vis/NIR light compared to pristine anatase TiO₂ or air-passivated Ti NPs. In addition, Ti@TiO₂ NPs show strong photothermal effect providing the most efficient H₂ production under the joint effect of light and heat. The apparent activation energy $E_a = 27$ kJ·mol⁻¹ assumes that the thermal effect of H₂ generation is governed by diffusion of intermediates. Suggested reaction mechanism involves nonradiative Landau damping, resulting in the excitation of energetic electrons and holes in the metal particle, electron holes accumulation in a semiconducting TiO₂ shell via charge separation and multiple charge-transfer steps. The photoluminescence of TiO₂ originated from electron-hole recombination is completely quenched in the case of Ti@TiO₂ NPs indicating effective charge separation. In principal, Ti@TiO₂ photocatalyst has the same potential areas of applications as TiO₂/Pt photocatalyst.

Abstract ID: 164

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Chemistry of 2D Materials for Energy, Catalysis and Sensing Applications

Keywords: WS₂, dichalcogenides, exfoliation, gas sensors

Controlling microstructure and surface oxidation of few layers exfoliated WS₂ for NO₂ and H₂ gas sensing applications

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WS₂ exfoliated by a combined low energy ball milling and sonication technique to produce mono to few-layer WS₂ with controlled morphology and chemical composition is characterized and assembled as chemo-resistive NO₂, H₂ and humidity thin films sensors. Microstructural analyses of exfoliated WS₂ reveal flakes with average dimensions of 110nm, “aspect ratio” of lateral dimension to the thickness of 27. Due to spontaneous surface oxidation of exfoliated WS₂ to amorphous WO₃, films have been pre-annealed at 180°C to stabilize the WO₃ content. Microstructural characterization by XPS, Raman and grazing incidence XRD techniques, highlighted the formation of \approx 58% amorphous WO₃ on the surface of the pre-annealed 180°C WS₂ flakes. XPS and XRD analysis repeated after one year conditionings highlighted that amorphous WO₃ concentration is stable, attesting the validity of the pre-annealing procedure. WS₂ films were NO₂, H₂ and humidity tested at 150°C OT, exhibiting experimental detection limits of 200 ppb and 5 ppm to NO₂ and H₂ in dry air respectively, and reasonably good relative response in the 10%-80% Relative Humidity (RH) range. Long term stability of the electrical response recorded over one year of sustained conditions at 150°C OT and different gases demonstrated good reproducibility and stability of the electrical signal. The role played by WO₃ as respect to WS₂ upon gas response has been addressed and a likely reaction gas-mechanism presented. Controlling the microstructure and surface oxidation of exfoliated transition metal dichalcogenides represents a stepping-stone to assess the reproducibility and long-term response of TMDs monolayers in gas sensing applications.

Key Words: Dichalcogenides, WS₂ exfoliated, gas sensors

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Thursday, 22/Aug/2019 9:48am - 10:00am

Abstract ID: 165 / FLNM: 10

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Photonic and optoelectronic device applications of low dimensional, nano and 2D materials

Keywords: Electrochromism, Nanoparticle, Smart Windows

Single nanoparticle electrochromism measurements reveal heterogeneous coloration rates and ion trapping sites in smart windows

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Developing large area electrochromic smart windows based on nanoscale materials demands that trillions of nanoparticles modulate between transparent and colored states at the same rate. However, it is unclear how nanoparticle heterogeneity contributes to variable coloration dynamics. Here we demonstrate a single nanoparticle electrochromism approach to study optical modulation rates upon lithiation of isolated, clustered, and thin film tungsten oxide nanorod electrodes. We observe a particle-dependent waiting time for coloration (from 100 ms to 10 s) due to Li-ion insertion at optically inactive surface sites. Longer nanorods achieve higher OD modulation than shorter nanorods because they develop a Li-ion gradient that increases from the nanorod ends to the middle. Interestingly, electrochromic irreversibility increases monotonically with the number of particle-particle interactions due to ion trapping at nanoparticle interfaces. These findings lead us to propose a nanostructured electrode architecture that optimizes coloration magnitude, rate, and reversibility across large area electrochromic smart windows.

Abstract ID: 166**Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)****Oral Presentation***Topics:* Applications of low dimensional, nano and 2D materials*Keywords:* TMD, photovoltaics, photocurrent microscopy**Efficient Carrier Collection in Monolayer Liquid Junction Photovoltaic Systems****Justin Sambur**Colorado State University, United States of America; jsambur@colostate.edu

Solid state photovoltaic devices made of two-dimensional (2D) transition metal dichalcogenide (TMDs) monolayers such as WSe₂, MoS₂, and MoS₂/WSe₂ have achieved 1-3% power conversion efficiency. However, photo-generated charge carriers in the middle of the device typically traverse tens of micrometers toward end-on electrical contacts at the device edge. The long transport distances parallel to the TMD layers give rise to transport-limited device physics that limit overall device performance. Here we demonstrate ultrathin liquid junction photovoltaic systems that use an iodide-based hole-selective electrolyte contact that facilitates a charge transport pathway perpendicular to the 3-atom thick TMD materials. These proof-of-concept indium doped tin oxide (ITO)|monolayer TMD|I⁻/I₂|Pt cells exhibit peak internal quantum efficiencies (IQE) of 7.1%, 34.5%, and 8.2% and open circuit voltages (VOC) of 0.46 V, 0.26 V, and 0.28 V for WSe₂, MoS₂, and MoS₂/WSe₂ heterojunctions. The photocurrent efficiency values are competitive with solid state devices. Surprisingly, we observe a non-linear scaling relation between IQE and layer thickness for homojunction and heterojunction TMDs that can be attributed to either thickness-dependent charge carrier dynamics or a buffer layer screening effect at the ITO/TMD interface. We discuss opportunities to improve the fill factor and VOC by interface engineering and tuning the energy level offset between the TMD composition and redox electrolyte potential.

Thursday, 22/Aug/2019 8:00am - 8:12am

Abstract ID: 167 / FESC: 1

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: Hydrogen evolution reaction, PbS nanocrystal, Anatase TiO₂ microsphere, Broadband harvesting, Near-infrared response

Enabling Low Energy Photons Harvesting for Efficient H₂ Production Employing PbS Nanocrystals Modified Anatase TiO₂ Microspheres

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Since the pioneering work on photosplitting water over TiO₂ electrode was reported in 1972,¹ photocatalytic H₂ production technique was thought as a potential approach to solving the current energy pinch, and therefore various semiconductors have been explored to act as photocatalysts.^{2,3} Among which, TiO₂ with a wide bandgap (~3.20 eV) is the most extensively investigated UV-responsive photocatalyst. Nevertheless, UV rays ($\lambda < 400$ nm) only accounts for ~4% of the total solar spectrum (AM1.5G), while visible light (400 nm $> \lambda < 800$ nm) and infrared rays ($\lambda > 800$ nm) account for ~53% and ~43%,² respectively. Therefore, an ideal photocatalyst should be capable of utilizing low energy photons in visible (Vis) and/or near-infrared (NIR) regions to maximize its use of naturally available sunlight.

Infrared-bandgap PbS quantum dots have been extensively used in solar cells for an extraordinary conversion efficiency,⁴ but its direct application in photocatalytic system for utilizing the low energy photons of solar spectrum is rare.^{5,6} In this context, PbS nanocrystals (NCs) are used to modify anatase TiO₂ microspheres (AMS) to fabricate a novel PbS/AMS heterostructure enabling visible (Vis) and near-infrared (NIR) light harvesting for efficient H₂ production for the first time. Due to the AMS with three-dimensional network-like structure acting as the support of intimately contacted PbS NCs, the hot electrons of PbS can inject into AMS before the thermalization losses. As expected, the PbS/(Pt-AMS) exhibits H₂ production activity of 813 $\mu\text{mol h}^{-1}$ under UV-Vis-NIR light irradiation with apparent quantum yields of 38.6%, 26.2%, 2.43%, 3.21%, 2.17%, 0.36%, 0.11% and 0.01% illuminated at 350, 420, 550, 700, 760, 850, 950 and 1064 nm monochromatic light, respectively. The present results can lead to intriguing applications of infrared-bandgap materials enabling broadband harvesting for efficient H₂ production.

Thursday, 22/Aug/2019 8:00am - 8:12am

Abstract ID: 168 / FLNM: 1

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Advances in the Synthesis and Characterization of low dimensional, nano and 2D materials

Keywords: MAXenes, MABenes, 2D Particles

Design of Novel Particulates from MAX and MAB Phases

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MAX Phases are novel ternary carbides and nitrides bestowed with exciting properties. MAB Phases are recent addition to the family of these ternary solids. In this paper, we report the design of novel particulates from MAX and MAB Phases. More particularly, I will present some of the recent studies in my lab on the design of novel particulates by etching MAX and MAB Phases. As background, numerous studies have reported MXenes by completely etching A-group element from MAX Phases but there has been limited studies on the design of novel compounds by retaining controlled amount of A-group elements inside the MAX or MAB Phase lattice structure.

Abstract ID: 169 / Poster: 36

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Nanogenerators and self-powered nanosystems

Keywords: micromotors, glucose, visible light, Cu₂O, N-CNTs

Glucose-Fuelled Photocatalytic Micromotors

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Synthetic glucose-fuelled micro/nanomotors, which hold great promise in various applications, have been widely investigated in recent years. However, currently, all of the glucose-fuelled micro/nanomotors are driven by enzyme-catalytic driven mechanisms and usually suffer from strict operated conditions and weak propulsions which greatly limit their applications¹. Here, we report the fastest glucose-fuelled cuprous oxide@N doped carbon nanotube (Cu₂O@N-CNT) photocatalytic micromotor. We firstly use photocatalytic reactions instead of enzymatic reactions to decompose biocompatible glucose so as to generate sufficient energy for efficiently propelling micro/nanomotors, and such photocatalytic methods are extremely efficient, stable and easy operated compared to previously reported enzymatic ways. To the best of our knowledge, the Cu₂O@N-CNT micromotors are the most powerful glucose-fuelled micromotors up to now, the speed can reach up to 18.71 $\mu\text{m/s}$, which is comparable to conventional Pt-based catalytic Janus micromotors usually fuelled by toxic H₂O₂ fuels². In addition, such micromotors are the fastest photocatalytic micromotors which can be operated in fully green environments so far. The speeds of motors are almost 12 times fast than that of previous reported visible light-driven micromotors (around 1.61 $\mu\text{m/s}$) in pure water³. Furthermore, the velocities of such motors can be efficiently regulated by multiple approaches, such as adjusting the N-CNTs contents within the micromotors, glucose concentrations or light intensities. Finally, the Cu₂O@N-CNT micromotors exhibit highly controllable negative phototaxis behavior (moving away from light source) due to their unique light-induced self-diffusiophoretic propulsion mechanism, thus, their directions can be precisely controlled by regulating the light sources positions. Such motors with outstanding propulsion in biological environments, and wireless, repeatable, light-modulated three dimensional motion control are extremely attractive for future environmental and biological applications.

Abstract ID: 170

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Photocatalytic and electrochemical water splitting

Keywords: Attapulgite; g-C₃N₄; Visible light photocatalysis; Ag; Reaction mechanism

Synthesis of nano-Ag-assisted attapulgite/g-C₃N₄ composites with superior visible light photocatalytic performance

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Graphitic carbon nitride (g-C₃N₄) based hybrid photocatalysts have recently emerged as a new class of functional materials for solar energy conversion. Here, we synthesized a novel visible-light-responsive Ag-assisted attapulgite/g-C₃N₄ composite photocatalyst (ATP/g-C₃N₄-Ag) by depositing Ag nanoparticles onto the surface of ATP/g-C₃N₄, which is fabricated by introducing a thin layer of g-C₃N₄ onto the ATP surface (pre-grafted by (3-glycidyloxypropyl) trimethoxysilane (KH560)). The products were fully characterized by XRD, FT-IR, BET, XPS, UV-vis TEM and Raman techniques. Results show that g-C₃N₄ thin layer is uniformly loaded onto the ATP surface by forming a new chemical bond (Si-O-C), which results from the bimolecular nucleophilic substitution reaction (SN₂) between KH560 and melamine. Comparing with g-C₃N₄ and ATP/g-C₃N₄, ATP/g-C₃N₄-Ag exhibits remarkably enhanced visible light photocatalytic activity in degradation of methyl orange (MO). The highest decomposition rate of MO reaches 96.70% within 20 min, which remains unchanged after 4 cycles. The possible photocatalytic mechanism is investigated by photoluminescence, electrochemical impedance spectroscopy analysis, and radical trapping experiments. Results suggest that •OH and •O₂⁻ are the main active species, and numerous electrons on the Ag surface will be utilized to generate considerable amount of •O₂⁻ and •OH for the degradation of MO.

Abstract ID: 171

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: waxy crude oil, pour-point depressant, nanohybrid materials

The effect of nanohybrid materials on the pour-point and viscosity depressing of waxy crude oil

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The flowability of waxy crude oil has been always a problem in the field of gas and oil storage and transportation both in China and other countries. In this research, a kind of novel nanohybrid pour-point depressant (PPD) composed of organic modified montmorillonite and Ethylene Vinyl Acetate (EVA) was applied to the pour-point and viscosity depressing of waxy crude oil. The results showed that the viscosity and pour point of waxy crude oil was sharply decreased, and the long-term stability of nanohybrid PPDs was superior to the conventional EVA PPDs. POM and XRD were utilized to study the effect of nanohybrid PPDs on the crystallization of crude oil. The incorporation of nanohybrid PPDs resulted in the improvement of the crystal structure and crystallization behavior: the amount of wax crystals decreased and the wax crystals were not easy to be entangled. And the temperature at which crude oil started to crystallize was lower. The excellent pour-point and viscosity depressing effect was firstly discovered in this study and industrially applied to some pipelines of PetroChina, which is of great importance to the safety, efficiency and energy-saving of waxy crude oil transportation.

Abstract ID: 172

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Electrochemical Supercapacitors

Keywords: Porous carbon, Supercapacitor, Energy Storage

Doped porous carbon for high performance supercapacitors

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Porous carbon-based nanomaterials such as graphene, carbon nanotubes, carbon nanosheets and carbon nanosphere are still the first choices for fabricating the electrodes of supercapacitor because of their excellent stability, good conductivity, and large surface area . However, the capacitance of carbon based materials is intrinsically low, which limit their wide application. Doping carbonaceous materials with a conducting polymer or transition metal compounds to generate pseudocapacitance is effective way to improve their electrochemical performance. In this study, porous carbon was functionalized with transition metal oxides, conducting polymer and heteroatom for the purpose of supercapacitive enhancement. The electrochemical performance of the supercapacitor was studied in details.

Abstract ID: 173

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Invited Talk

Topics: Bio-inorganic nanomaterials

Keywords: DNA nanotechnology, plasmonics, nanoparticle chain waveguide, electron energy loss spectroscopy, cathodoluminescence imaging spectroscopy, fluorescent nanodiamonds

DNA-assembled Plasmonic Waveguides for Nanoscale Light Propagation to a Fluorescent Nanodiamond

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Plasmonic waveguides consisting of metal nanoparticle chains can localize and guide light well below the diffraction limit, but high propagation losses due to lithography-limited large interparticle spacing have impeded practical applications. We demonstrate that DNA-origami-based self-assembly of monocrystalline gold nanoparticles allows the interparticle spacing to be decreased to ~ 2 nm, thus reducing propagation losses to 0.8 dB per 50 nm at a deep subwavelength confinement of 62 nm ($\sim \lambda/10$). We characterize the individual waveguides with nanometer-scale resolution by electron energy-loss spectroscopy. Light propagation towards a fluorescent nanodiamond is directly visualized by cathodoluminescence imaging spectroscopy on a single-device level, therefore realizing nanoscale light manipulation and energy conversion. Simulations suggest that longitudinal plasmon modes arising from the narrow gaps are responsible for the efficient waveguiding. With this scalable DNA origami approach, micrometer-long propagation lengths could be achieved, enabling applications in information technology, sensing and quantum optics.

Abstract ID: 174

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: Waterborne polyurethane conductive composite coating, Multiwalled carbon nanotubes, Resistivity, Corrosion rate, Bond strength

Preparation and properties of an eco-friendly polyurethane conductive composite coating modified with MWCNTs

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Owing to emitting many volatile and flammable solvents during the process of preparation and construction, oil coatings are easy to catch fire, generally leading to potential safety problems. Therefore, waterborne coatings using water as a dispersion medium will become one of the main anticorrosive coatings in the future. A kind of eco-friendly MWCNTs/WPU conductive composite coating, based on the eco-friendly waterborne polyurethane (WPU) as a film-forming material and multiwalled carbon nanotubes (MWCNTs) as a conductive medium, was prepared in this work. The electrical conductivity and corrosion resistance of the composite coating, and its bond strength to steel substrate were respectively investigated. The results indicated that, when the content of MWCNTs increased, the electrical conductivity of the MWCNTs/WPU composite coating was greatly improved, however, its bond strength to Q235 steel substrate and corrosion resistance were decreased slightly. When the content of MWCNTs was 0.6 wt.%, a conductive network was formed in the composite coating. 0.6 wt.% MWCNTs/WPU conductive composite coating with a relatively high resistivity of 12845 $\Omega \cdot m$ began to conduct electricity. Its corrosion rate was 0.061799mm/a, 37 times lower than that of the uncoated Q235 steel substrate, resulting in good corrosion resistance. Its bond strength to Q235 steel substrate was 3.03 MPa. This work may provide a theoretical basis for preparation of an eco-friendly polyurethane conductive coating and protection of the equipment used in the field of oil field and oil refinery.

Thursday, 22/Aug/2019 9:24am - 9:36am

Abstract ID: 175 / FLNM: 8

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nanomaterials for Biomedical Applications

Keywords: silver clusters, lipoic acid, antibiotic, electrospray ionization mass spectrometry

Super Atom Complexes with Antiviral and Bactericidal Activity

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In 1982, Dr Jim Hainfeld demonstrated that a gold-cluster (Au₁₁(PPh₃)₇I₃) could be obtained in a water-soluble form and modified by conjugation of the Ph*⁻groups to biomolecular groups.^{1,2} This molecule has enhanced stability because its 8 "free" electrons occupy a closed-shell S₂P₆ configuration of globular 'super-atomic' orbitals.³ Thus developed the new field of TEM/X-ray diagnostics and therapeutics based upon conjugation of noble-metal (gold) 'superatom complexes' to biologically active agents.

Along those lines, we report a promising development using an exceptionally stable silver (Ag₂₉) cluster and 12 lipoic acid ligands.⁴ The pendant carboxylates of each ligand is covalently coupled (conjugated) to β -lactam penicillanic acid derivatives. The antimicrobial activity of the cluster is demonstrated by various spectroscopic methods including HPLC-ESMS (Figure 1), UV-VIS, FTIR, Raman, NMR, XRD, and STEM (Figure 2). The efficacy of the conjugated cluster against Methicillin-Resistant Staphylococcus aureus bacteria (MRSA) and preformed Candida albicans fungal biofilm, exceeds that of its constituents thus demonstrating a synergetic effect.

Figure1: Electrospray ionization mass spectrometric analysis of the conjugated Ag₂₉ lipoate complex in solution.

Figure 2. SEM images showing effect of cluster on a preformed biofilm of Candida albicans and MRSA colonies. Before: a) & c). After: b) & d).

Key Words: silver clusters, lipoic acid, antibiotic, electrospray ionization mass spectrometry

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Abstract ID: 176 / Poster: 44

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Biodetection

Keywords: Nanoporous, Monolayer, Carbohydrate, Glycoprotein, Biosensor

Recent Applications of Nanoporous Gold to Glycoscience

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Nanoporous gold (np-Au) has become a widely studied nanomaterial due to its many versatile formats, high and tunable surface area, tunable pore dimensions suitable for accommodation of biomolecules, chemical stability, capacity for surface modification, and potential usage in biotechnology applications. The field of glycoscience is growing in significance as the importance of glycans in human health and disease becomes more fully understood at the molecular level. np-Au can be applied to a number of needs in the field of glycoscience. Our lab has applied np-Au to applications in glycoscience including the capture and release of glycoproteins, and the detection of glycoprotein interactions by using either electrochemical methods or localized surface plasmon spectroscopy (LSPR). The capture of glycoproteins onto high surface area np-Au is demonstrated using both lectin-glycan interactions and also interaction between glycoproteins and np-Au modified with boronic acid functional groups. Thermogravimetric analysis and use of a uv-visible HPLC detector in a flow cell containing monoliths of np-Au are applied to monitor capture of glycoprotein and its elution by flow of free ligand. The modification of np-Au by self-assembled monolayers (SAMs) with terminal boronic acid groups has been used together with LSPR to monitor the capture of glycoprotein by the induced shift in the LSPR peak wavelength. Square-wave voltammetry methods can also be applied to monitor the binding of glycoproteins to np-Au modified either by SAMs with terminal boronic acid groups or by conjugated lectins.

Thursday, 22/Aug/2019 11:24am - 11:39am

Abstract ID: 177 / FLNM-2: 3

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Keynote

Topics: Structural, Electronic, Optical and Magnetic Properties

Keywords: Self-assembly, Fluorescence, Molecular-recognition.

Emission Properties of Organic Fluorophores in Solid and Solution

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Emission Properties of Organic Fluorescent Molecules in Solid and Solution

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Organic fluorescent molecules provide scopes to study their emission properties in solution as well as in solid state. Electronic, steric and conformational arrangements in these states can be varied to implicate their effects in the respective emission property. In many cases the emissions shown by a compound in solid-state widely differs from the emission shown in the solution. Such changes occur due to the changes in emission paths by changing structural parameters by adjusting orientations, hydrogen bonds, complexation, confinements etc. Each of them has a role to influence the mechanism of emissions. In certain cases, the extent of tautomers in solution differs from the one observed in solid to influence the emissions by influencing excited state intramolecular proton-transfer. Series of poly-aromatic fluorescent molecules will be presented to establish the differences in optical properties in solution properties from the one observed in solids. Mechanistic aspects through analysis of quantum yields, life-time decay profiles and structural studies in solution and solid state will be presented. The utility of such processes in molecular-recognition, ion-recognition, modulation of emissions, dual emissions will find priority in the discussion.

Key Words: Self-assembly, Fluorescence, Molecular-recognition.

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Abstract ID: 178 / Poster: 40

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Environmental biosensors

Keywords: Silica, Nanoparticles, Nanopores, Hexavalent Chromium, Adsorption

Chemically functionalized amorphous silica nanoparticles equipped with uniform nanopores for removing hexavalent Chromium ions from wastewater

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Silica is a mineral frequently found in nature and has been widely employed in industrial fields. In particular, amorphous silica nanoparticles (ASNs) are one of the most common nanomaterials being used in many applications including industrial manufacturing, composite materials, cosmetics, and foodstuffs due to their favorable physic-chemical properties. Because of their facile synthesis, relatively easy surface modification and labeling, and good biocompatibility, ASNs have many possible uses in biomedical and pharmaceutical areas such as drug delivery and therapy, multifunctional bioimaging probes, biosensors, etc. We developed synthetic methods to prepare highly monodisperse (<10%) ASNs with the averages sizes ranged from ~15 to 300 nm. Furthermore, our methods enable us to prepare highly monodisperse mesoporous silica nanoparticles (MSNs) with the averages sizes ranged from ~20 to 100 nm by introducing uniform nanopores of less than ~3 nm formed inside the ASNs. By systematically tailoring the MSNs' porosity and chemically functionalizing MSNs with amino (NH₂-) group, adsorption of hexavalent Chromium (Cr(VI)) ions in aqueous environments is significantly enhanced to deliver high loading and removal efficiency of Cr(VI) ions. In the end, our study offers a facile and promising means to efficient removal of heavy metal ions from wastewater environments. Our results on the complete characterization of NH₂-functionalized ASNs and MSNs and the quantitative analysis of Cr(VI) adsorption and removal processes including its adsorption kinetics will be discussed in the presentation.

Abstract ID: 179

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Anti-cancer therapy

Keywords: Intracellular self-assembly, Drug Resistance, Modification of Chemotherapeutic Drugs, Reactive Oxygen Species

In Situ-Induced Multivalent Anticancer Drug Clusters in Cancer Cells for Enhancing Drug Efficacy

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Increasing intracellular drug concentration is an effective way for cancer chemotherapeutics to enhance efficacy and combat drug resistance. In this work, we prepared a series of anticancer drug conjugates by linking thiol-modified oligo(p-phenylene vinylene) and paclitaxel, vincristine, teniposide, tamoxifen, doxorubicin or podophyllotoxin (OPV-S-drugs) through Michael addition reaction. These OPV-S-drugs could undergo intracellular assembly and aggregation upon oxidation to yield multivalent anticancer drug clusters, which inhibited their diffusion from cancer cells. The in-tracellular aggregation of OPV-S-drugs originates from π - π stacking and hydrophobic interactions between OPV backbones, followed by the crosslinking via thiol-thiol bond formation in the presence of reactive oxygen species (ROS). The drug clusters only occur in the cytoplasm of cancer cells possessing higher expressing level of ROS, but not in healthy mammalian cells, thus reducing the cyto-toxicity to normal cells. Specially, the super-toxicity of podophyllo-toxin on normal cells was obviously suppressed while the drug efficacy was kept through our new strategy. The diverse action mechanisms of OPV-S-drugs towards cancer cells were proposed.

Abstract ID: 180

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Composites in Innovative Applications

Keywords: Metal Detection, Surface Plasmon Resonance

Rapid Detection of Hg using Ag Incorporated Recycled Paper

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Heavy metal contamination in water and other ecosystems is one of the major environmental issues and has gained significant attention. Mercury ion (Hg^{2+}) arising from a variety of natural sources and industrial wastes has been widely recognized as one of the most hazardous pollutant. It is very important to develop highly selective and sensitive probe for rapid detection of Hg^{2+} in aquatic ecosystems. The present study is an attempt to develop a metal detecting paper. The detection of Hg^{2+} is mediated by the surface plasmon resonance of silver nanoparticles. An ecofriendly approach has been used to develop the sensor using recycled paper. The AgNPs incorporated recycled paper has been used for detecting Hg metal ions upto 10^{-6} moles in aqueous system. In addition to high selectivity and sensitivity towards Hg^{2+} , the recycled exhibited antimicrobial as well as photocatalytic properties.

Abstract ID: 181

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Advanced Numerical Techniques

Keywords: Fibre-reinforced composite panels, Low-velocity impact, Load-deflection, Absorbed energy

Low-velocity impact-induced damage and failure prediction of fibrous composite panels using data filtering, load-deflection, and absorbed energy approaches

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This work is concerned with flat nose-shape low-velocity impact-induced damage and failure predictions of fibrous composite panels. Fibrous composite aerospace structures are exposed to drop weight impacts during part assembly, maintenance, and service life. Such impact inflicts invisible internal damages that cannot be detected during routine inspections, but the damages could cause unexpected catastrophic failure of the structures during future operations. Extensive studies are being conducted to improve damage resistance and damage tolerance capabilities of the structures to prevent unexpected failures, to save human lives, and capital assets. Previous studies on the topic reveal that load-deflection and absorbed energy based approaches work well for onset of the impact-induced damage. However, flat nose impacts of relatively thick laminates produce level off load-deflection curves once certain displacement/energy level is reached. Little information can be extracted about the internal damage progression and ply-level failure mechanisms using the conventional approaches. Advanced data filtering techniques are required to complement such approaches to correlate load drop thresholds to damage zones and quantify different ply-level failure mechanisms. In the current work, test generated data was filtered, and correlated to load drops with load-deflection curves, and areas under the curves are numerically integrated to approximate the absorbed energy profile diagrams to predict and quantify different failure mechanisms. Implementation of the data filtering to the data obtained from flat and round nose impacts of 8- and 16-Ply panels reasonably predicted ply-level failures. Comparisons of the results to the available data in the literature shown that the combination of data filtering techniques, load-deflections, and energy-based approaches are found to be more suitable for the determination of initiation, propagation, accumulation, extent of impact-induced internal damage, and ply-level failure mechanisms.

Abstract ID: 182**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Anodes and cathodes Materials

Keywords: Silicon, Nano, Energy Storage

Synthesis of Nanomaterials for Energy Applications on the pilot-plant scale: Energy Storage

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Nanostructured silicon has been identified as a promising material for a wide variety of energy-related applications such as thermoelectrics and lithium ion batteries. Especially the mechanical strength of nano silicon is of high importance for battery applications due to the enormous change in volume during charge and discharge. Theoretical as well as experimental results confirm that particle sizes below 200 nm are highly advantageous for long-term stability of silicon-based electrodes. To further investigate the properties and applicability of this material, the demand for larger amounts of silicon nanoparticles increases. Gas phase synthesis is in general a well-suited method to provide large amounts of nanoparticles in reproducible and high quality. However, up-scaling of well-studied laboratory scale syntheses methods is still a challenge due to different scaling laws. We investigated the scale-up of silicon nanoparticle synthesis in a hot-wall and a microwave supported plasma reactor and generated highly sophisticated materials for the use in lithium ion battery applications.

The silicon nanoparticles are synthesized by thermal dissociation of the gas-phase precursor monosilane (SiH₄). In the hot-wall reactor, pyrolysis is done using convective heating between 1000 and 800°C producing either crystalline or amorphous material, respectively. The process pressure can be varied between 15 and 100 kPa. The particles are collected on a filter membrane and subsequently detached from the membrane by a back-pressure impulse. Finally, the nano-sized material is packed under inert gas in sealed bags. Depending on the precursor concentration, production rates up to 1 kg/h can be applied.

In the microwave plasma reactor, crystalline silicon nanoparticles are produced by decomposition of SiH₄ in the plasma zone using a microwave frequency of 915 MHz and a microwave power of up to 50 kW. We investigated the influence of different process conditions such as precursor concentration and gas velocity on nanoparticle properties such as particle size and morphology. Typically, silicon nanoparticles from the plasma reactor are spherical, highly crystalline and mostly don't show any hard agglomerates due to Coulomb repulsion during particle formation. Production rates up to 0.3 kg/h could be realized [1]. Both reactors are able to produce silicon nanoparticles with mean particle diameters well below 200 nm. They were tested for long term production for 36h (hot-wall) and 8h (plasma) as well as for reproducibility. In each case, ex-situ analysis revealed the reproducible production of morphologically identical materials. Electrochemical testing showed that the silicon nanoparticles synthesized exhibit a superior long-term stability in lithium ion batteries.

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Abstract ID: 183

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Thin films for optoelectronics, nanoelectronics and spintronics

Keywords: Thin films, Gold, Flexible Electronics, Transparent conductive oxide

Characterization of ITO & Gold Thin films on Novel Flexible PDMS substrate for Flexible Electronic Devices

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Flexible Organic Electronic Devices (OEDs) have numerous applications in our day to day life owing to advantages such as ease of processability, potentially low cost, high throughput, and large-area roll-to-roll fabrication techniques. In this regard, a new attempt to develop flexible devices using flexible PDMS substrate is reported in this paper. For the development of flexible devices, a transparent and conductive oxide is to be coated which acts as a backbone for the entire device. In connection to this, deposition and characterization of indium tin oxide (ITO) and Gold (Au) on the fabricated flexible PDMS substrate is carried out and reported. ITO layers are coated using RF and DC sputtering methods and characteristics such as transmittance, resistance and adhesion are reported. As a next attempt to improve the efficiency of the device, the Au layers are coated on the PDMS substrate and the same characteristics are analyzed and reported. Compared to ITO, Au layer has better properties on the flexible PDMS substrate. Further to improve the adhesion between the Au layer and the PDMS substrate, the surface modification of the PDMS substrate is carried out using ozone treatment followed by Sodium Dodecyl Sulfate (SDS) and the characteristics of the same are found to be improved. The deposited layer has good transmittance, conductivity and adhesion with the PDMS substrate. The deposition of these thin films in the flexible substrate will pave a path for the fabrication of flexible electronic devices and circuits with high efficiency.

Abstract ID: 184

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Nano and Environmental catalysis

Keywords: PS-HDODA, catalysis, metal nanoparticles

Catalytic activity studies of Metal Nanoparticles supported on a novel functional organic polymer

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Polymer metal complex is mainly composed of a synthetic polymer and a metal ion. Its synthesis represents an attempt to give an organic polymer inorganic function. A novel polymeric support polystyrene cross linked with 1, 6-hexanediol diacrylate (PS-HDODA) with improved swelling and solvation properties is introduced for heterogeneous catalysis. This flexible support with optimum hydrophobic–hydrophilic balance could be easily functionalized. Metal and metal nanoparticles could be easily stabilized for catalytic activity by incorporating into the functionalized PS-HDODA resin by using various methods. The efficiency of this new support in heterogeneous catalysis is established by conducting various reactions with high efficiency. Metal nanoparticles could be easily and safely dispersed into this polymeric hydrogel for enhanced catalytic activity. To exemplify the advantages of this new resin in catalysis different transition metals like Co(II), Zn(II) and their nanoparticles were attached to the functionalized polymer and were tested for various reactions. This study offers a promising route in catalyst design and its applications in heterogeneous catalysis.

Abstract ID: 185

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nanomaterials for Energy and Environmental Applications

Keywords: Plasmonic, Photocatalysis, Nanoparticles, Plasma

Plasmon-induced chemistry with plasmonic titanium nitride nanoparticles as an alternative to gold

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The light-harvesting capacity of plasmonic nanoparticles has recently garnered attention in the synthesis of nanoantennas for photocatalysis. Aluminum, gold, and silver have been used to successfully drive hydrogen dissociation and CO oxidation reactions by injecting hot electrons into chemically active catalysts —such as platinum and palladium— adsorbed to their surface. However, the low response of aluminum at visible-near infrared (NIR) wavelengths, the high cost of silver and gold, and the low thermal stability of these three metals, inspire the quest for alternative plasmonic materials that could potentially expand the field towards more ambitious and cost-effective applications. Titanium nitride (TiN) is a conductive ceramic with high hardness and bulk melting point (2930 °C). Its plasmon resonance located in the visible-NIR region, low cost relative to gold and silver, and well-understood properties as a thin film in the semiconductor industry make it a strong alternative to mainstream plasmonic metals. The present work encompasses a comprehensive study of the oxidation kinetics of TiN particles at the nanoscale and an exploration of its role as nanoantennas for light-induced methanol reformation. TiN particles are synthesized via a scalable, modular, non-thermal plasma method. Titanium and nitrogen precursors are transported into a RF frequency plasma where TiN particles nucleate and grow. Platinum nanoparticles were subsequently deposited on the TiN by photo-induced reduction of an aqueous solution of chlorplatinic acid. The reduction of the precursor metal was driven by electron hole pair generation via plasmon decay. The addition of methanol as a hole scavenger increased the electron lifetime, leading to the obtention of metallic platinum. This reaction occurred at temperatures below 40°C under visible light illumination. The results were corroborated by X-ray Photoelectron Spectroscopy (XPS) and UV-vis spectrophotometry measurements. In addition, the photocatalytic properties of TiN/Pt catalysts were further evaluated for the methanol reformation reaction. This work strengthens the case for alternative plasmonic materials in a field dominated by precious metals.

Abstract ID: 186

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Advances in the Synthesis and Characterization of low dimensional, nano and 2D materials

Keywords: Graphene oxide, electrochemical exfoliation, current density

Synthesis and characterization of high aspect ratio graphene oxide through a continuous re-exfoliation of graphite

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Graphene oxide was synthesized using electrochemical exfoliation of graphite with different bulk densities. A facile system was developed such that a continuous exfoliation and re-exfoliation of graphite could be achieved. Parameters were optimized like, ratio of electrolyte constituent H₂SO₄ to NaOH, current, voltage, distance between two electrodes to achieve a continuous synthesis of graphene oxide. Structural and chemical characterization was carried out using Raman Spectroscopy, Transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), X-ray Diffraction (XRD). From TEM images it was observed that the composition of electrolyte affected the no of layers and lateral dimension of graphene oxide sheets. Lateral dimensions of graphene oxide sheet observed were ranging from 5 to 25 microns having a thickness of single as well as few layers. The yield of graphene oxide was also affected by the current density. The oxygen functionality and crystallinity were determined by XPS and Raman spectroscopy. By this method, a stable dispersion of graphene oxide in ethyl alcohol and water was obtained. This process has potential for scale-up and continuous production.

Keywords: Graphene oxide, electrochemical exfoliation, current density etc.

Wednesday, 21/Aug/2019 5:48pm - 6:00pm

Abstract ID: 187 / FBB-2: 10

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biomaterials for hard tissue applications

Keywords: Metallic implants, microstructure, biocompatibility, cytocompatibility, surface

Biocompatibility dependence of metallic biomaterials on microstructural mechanisms

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Biocompatibility of metallic biomaterials are investigated at several levels starting from their mechanical compatibility with the surrounding tissue, to their electrochemical stability when exposed to bodily fluids and their biocompatibilities at the in vitro and in vivo levels. Many factors contribute their biocompatibility response at these levels, including their chemical composition, presence of alloying elements, surface topography as well as their microstructures.

Effects of microstructural mechanisms on the material properties of metallic materials are usually explored with a focus on mechanical properties and deformation behavior. However, recent studies have shown that, microstructural properties of metallic materials can also be critical for determining their biocompatibility at different levels. For instance, ex situ biocompatibility is influenced by the presence of dislocations through localization of oxide particles around dislocation networks, which may affect ion release [1]. Moreover, surface topography is also affected by microstructure at the micro or nanoscale, which in turn affects cell attachment and proliferation behavior [2].

In the current study it is aimed to systematically investigate the effects of microstructural mechanisms on the cytocompatibility of metallic biomaterials.

With this motivation, 316L stainless steel, a widely known and conventional biomaterial used in orthopedic implants, will be investigated. Micro-deformation areas of various amounts and repeating orders will be formed on the surfaces of the stainless-steel samples, via the use of a micro-hardness testing devices. After examining the microstructural changes that formed in these areas through electron microscopy, the in vitro responses to these surfaces will be explored. For this purpose, osteosarcoma cells will be seeded on the samples with the introduced microstructures of various characteristics. Cell attachment and proliferation behavior of these cells on the various metal surfaces will be investigated through qualitative and quantitative analyses.

The outcomes of this study are aimed to shed light onto the main microstructural factors that affect the biocompatibility of metallic biomaterials and use the obtained knowledge in the design of novel bone implant materials.

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Abstract ID: 188

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Durability of composite materials

Keywords: Epoxy resin; Flake aluminum powder; Water aging; Strength loss

Effect of Water Uptake on the Mechanical Properties of Flake Aluminum Powder Filled Epoxy resin Composites

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Wide attention has been paid to epoxy resin in engineering fields due to its high strength, stiffness, electrical insulation and facile fabrication, etal. However, it was discovered that serious hydrothermal aging exits in epoxy, which compromises its normal service life . This work aims to improve water-heating aging of epoxy resin (EP). Flake aluminum powder (PAI) was incorporated in EP, then immersed in a water bath to study its effect on water aging of EP. After aging, the water diffusion in PAI/EP composites, containing 3wt.% PAI especially, obtained fairly improvement. In addition, the tensile and bending strengths of the EP were compromised from 29.9MPa and 60MPa, respectively, to 24.1 MPa and 49.8Mpa, respectively. However, the tensile and bending strengths of the sample with 3wt.% PAI were reduced from 45.0MPa and 118.8MPa, respectively, to 44.3MPa and 108.2MPa, respectively. Moreover, its bending and tensile strength losses with 1.6% and 8.9% exhibited the lowest in mechanical tests, which were lower than those of the EP by 91.8% and 47.6%, respectively. Thus, PAI not only is effective defences against water diffusion in EP, but also has effect on deflecting and pinning cracks to enhance strengths of composites.

Abstract ID: 189

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Photocatalysis

Keywords: Key Words: CH₃SH conversion pathway, g-C₃N₄/I₃⁻/I⁻-BiOI, Indirect Z-scheme, Interfacial charge transfer, Self-stabilized I₃⁻/I⁻

Self-Stabilized Indirect Z-scheme g-C₃N₄/I₃-BiOI for Highly Efficiently Photocatalytic CH₃SH Oxidation

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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. The g-C₃N₄/I₃⁻-BiOI composites, with heterojunction between porous g-C₃N₄ and BiOI ultrathin nanosheets, were firstly applied for the photocatalytic elimination 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 composition 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.

Wednesday, 21/Aug/2019 5:24pm - 5:36pm

Abstract ID: 190 / FCM: 8

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Analysis of composite beams, plates and shells

Keywords: Functionally Graded Materials, Composites, Vibration, Galerkin method, Power-Law distribution

Vibration Analysis of Functionally Graded Thin Plates with Linearly Varying Thickness using Variational Method

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Functionally Graded Composite Materials (FGMs) consist of two or more materials with continuously varying properties throughout the spatial profile. Typically, this grading is from a refractory ceramic to a metal. Such composites find uses in areas ranging from aerospace to medical applications. These applications require extensive study of the structural properties of FGMs. An analytical model has been developed in order to find the resonant frequencies of functionally graded thin plates with the help of variational Method. The classical plate theory has been used to formulate the properties of FGM plates. This model considers a linear variation in the plate thickness. The displacement functions have been derived through the product of a basis polynomial function and terms from Pascal's triangle. The boundary conditions taken into account are all sides clamped (CCCC) and all sides simply supported (SSSS). The power law distribution has been considered for the FGM property variation. The present study offers a simple analytical model for the vibration analysis of FGM plates while providing a valuable insight into the dynamic behavior for the same. This can further help in developing more dynamically durable FGM structures for applications such as automobiles and defense.

Abstract ID: 191

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Thermal problems on Composite structures

Keywords: Graphene, Copper, Coatings, Heat Transfer

Hierarchical Porous Graphene/copper composites for Enhanced Phase Change Heat Transfer Applications

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Owing to supreme thermal conductivity and wetting properties, graphene coatings have been exploited in numerous two-phase heat transfer applications such as electronics cooling, reboilers, refrigeration, and desalination. This talk will summarize various synthesis routes to obtain a variety of graphene/copper microscale and nanoscale surfaces while exercising control over deposition of number of graphene layers for boiling heat transfer studies. These surfaces were developed as benchmark studies, to produce a new class of hierarchical porous coatings to improve critical heat fluxes and heat transfer coefficients while facilitating morphology-induced mechanisms such as: wettability, contact angle hysteresis, roughness, and capillary wicking. In addition, the aging characteristics such as surface chemistry and morphology variability resulting from repetitive chaotic boiling tests will also be discussed.

Key Words: Graphene, Copper, Coatings, Heat Transfer

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Abstract ID: 192

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Environmental Catalysis

Keywords: Fe₃O₄ NPs; CS/Fe₃O₄ NCs; Photocatalytic degradation; Dye molecules.

Fabrication and characterization of chitosan/ferric oxide nanocomposites for photocatalytic degradation of important dye molecules

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Highly pure ferric oxide nanoparticles (Fe₃O₄ NPs) and chitosan/ferric oxide nanocomposites (CS/Fe₃O₄ NCs) were synthesized via one-step facile solvothermal method. The composition, structure, and morphology of the synthesized Fe₃O₄ NPs and CS/Fe₃O₄ NCs were characterized by Fourier transform infrared spectroscopy (FTIR), X-ray diffraction spectroscopy (XRD), thermogravimetric analysis (TGA), scanning electron microscope (SEM) and transmission electron microscopy (TEM). TEM images revealed that the Fe₃O₄ NPs possessed a sphere-like morphology and were homogeneously dispersed on the surface of chitosan film. The photocatalytic degradation of the synthesized CS/Fe₃O₄ NCs for rhodamine-B (Rh-B), methylene blue (MB) and methyl orange (MO) was evaluated under visible light irradiation. The irradiation time was varied based on the dye molecule (MB, MO and Rh-B) interaction with prepared Fe₃O₄ NPs and CS/Fe₃O₄ NCs. The dye molecule of Rh-B displayed superior photocatalytic execution than MB and MO. Therefore, the obtained CS/Fe₃O₄ NCs displayed advantageous photocatalytic degradation behavior for application in environmental remediation.

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Thursday, 22/Aug/2019 4:15pm - 4:27pm

Abstract ID: 193 / FESC-2: 12

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Nanostructured materials for advanced batteries

Keywords: Silicon, Nano, Energy Storage

A simple route for the synthesis of high-quality silicon-carbon composites for lithium-ion batteries

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Over the last decade, the research community engaged in significant efforts to develop silicon-based anodes and boost the energy density of lithium-ion batteries. [1] While, from a material engineering standpoint, silicon-carbon nanocomposites have been demonstrated as one of the most promising strategies to produce electrodes with long-cycle life, overcoming the problem of silicon swelling upon lithiation, synthesis methods suitable for the low-cost and large-volume production of these delicate nanoengineered structures have still to be demonstrated. In this contribution, we present two innovative simple, cost-effective and scalable-by-design methods that can potentially overcome the aforementioned limitations and pave the way for the introduction of silicon-based noncompounds into industrial manufacturing.

The first innovation is a method to produce silicon nanoparticles -NPs- with (i) high-purity (oxygen content <3%) and (ii) tailored nanoscale size [2]. The system comprises a non-thermal radiofrequency plasma reactor serially connected to a tubular furnace. The plasma discharge quickly converts a silicon containing gas into silicon NPs and ensures a high precursor utilization (over 90%). The aerosol is then seeded into the furnace where the NPs are sintered into larger structures at high-temperature. The final particle size can be precisely adjusted between 5 nm and 60 nm (size distribution within 10% of the average value) by simply changing the temperature of this second thermal stage (800-1000°C).

The second innovation is chemical vapor deposition -CVD- method that allows growing highly graphitized and conformal layers of carbon directly onto the surface of silicon NPs. The NPs are introduced into a hot-wall furnace with an alumina combustion boat and are wrapped with a conformal coating of amorphous carbon resulting from the dissociation of acetylene -C₂H₂- at 650 °C. After removing C₂H₂, the furnace is ramped up to 1000°C in Argon -Ar- yielding a controlled graphitization of the carbon-shell with no detectable presence of silicon carbide.

The combination of the two aforementioned approaches achieves the production of a battery grade silicon-carbon nanomaterial with tunable properties (i.e. size, graphitic carbon content and carbon shell thickness). The as-produced composite was tested in both half-cell and full-cell battery assemblies as a simple drop-in additive of graphite anodes. The addition of small amount of the Si-based active material (10% in wt) enables the fabrication of electrodes with a gravimetric capacity of 500 mAh g⁻¹, first cycle CE of 90% and stable cycling over 100 cycles.

Key Words: Silicon, Nano, Energy Storage

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Abstract ID: 194

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Magnetic film

Keywords: Exchange bias, perovskite thin films, RNiO₃, Metal oxides, Metal to insulator transition

Interfacial Ferromagnetism and Exchange Bias in NdNiO₃/NdMnO₃ Multilayers

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Abstract

Magnetic anisotropy at the interface between two layers results in to the phenomena of magnetic exchange bias [1]. The exchange bias resulting from interfacial coupling of layers is a key feature in the functionalities of modern spintronic devices [2]. NdNiO₃ and NdMnO₃ show antiferromagnetic order below $T_N \sim 200\text{K}$ and $T_N \sim 80\text{K}$, respectively, but we show that a multilayered structure of NdNiO₃/NdMnO₃ exhibits ferromagnetic exchange interactions between Ni and Mn ions at the interface. Due to the coexistence of two different magnetic orders with different transition temperatures in the same structure, exchange bias can be observed. We also show that the exchange bias can be influenced by parameters such as number of interfacial layers, strain and temperature in pulsed laser deposited (NdNiO₃/NdMnO₃)_n multilayers on [(LaAlO₃)_{0.3}(Sr₂AlTaO₆)_{0.7}] (LSAT) single crystal substrate. Here ‘n’ stands for the number of layers of each constituent material. Temperature dependent resistivity show first order metal to insulator phase transition ($\sim 200\text{K}$) for the top layer in these multilayered structures. For n=4, a large and negative horizontal exchange bias is observed at 25K [Fig. 1]. This effect decreases as temperature increases and it completely vanishes above 90K. A vertical shift in the magnetic hysteresis loop is also observed with field cooling [3,4,5].

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Abstract ID: 195 / Poster: 41

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Applications of Composites

Keywords: OSB, thermo-mechanical treatment, surface properties

Effect of Thermo-Mechanical Densification on Surface Properties of Commercial Oriented Strand Boards

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Commercial OSB composite was modified through the application of thermo-mechanical treatment (densification), being observed the behavior of its color, texture and wettability, aiming its usage at the furniture market. The colorimetry test was performed using a spectrophotometer, in accordance to the colorimetric parameters defined by CIELAB system proposed by Gonçalves (1993), the roughness test was performed using a rugosimeter, and the wettability test was performed using an optical contact angle goniometer. After the application of thermomechanical treatment, the OSB composite showed a darkening of its surface color, a behavior that was detected by the spectrophotometer, through the reduction in Lightness (L) parameter from 68.01 to 51.73, the increase in the green-red component (a^*) from 9.51 to 14.61, and the reduction in the blue-yellow component (b^*) from 33.09 to 31.62, representing a very appreciable color variation, turning from light-yellow (Control) to brownish-yellow (Densified). The surface of the OSB composite showed a significant reduction of its average roughness (R_a), from 7.70 (Control) to 5.15 (Densified), turning its surface plainer. As for the wettability, the water-contact angle presented a significant increase, from 85.99° (Control) to 97.19° (Densified), turning the OSB composite surface more hydrophobic. Hence, the proposed thermo-mechanical treatment was highly efficient to improve the surface of commercial OSB composite, allowing the furniture market to deliver a higher value-added product.

Thursday, 22/Aug/2019 4:51pm - 5:03pm

Abstract ID: 196 / FESC-2: 15

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Lithium Ion Batteries

Keywords: Rechargeable Battery, Lithium Ion Battery, Lithium Iron Phosphate Battery, LiFePO₄, Main Path Analysis

An Overview of Research on Lithium Iron Phosphate Battery

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This study aims to provide an overview on lithium iron phosphate (LiFePO₄, LFP) battery research with an emphasis on its recent research focus. LFP battery is suitable for electric vehicles owing to its good properties such as inexpensive, nontoxic, environmentally friendly, and thermal stability. Twenty-two years after Goodenough [1] proposed to use phosphor-olivines as positive-electrode materials, LFP battery remains a strong research topic. Over the years, the body of LFP literature has accumulated more than five thousand articles. Among them are review articles that report the progress of LFP. Each of these review articles is based on content reading and is usually technical oriented and focus on a specific subarea. With fast expansion of the LFP literature, it is getting more difficult to catch up with the overall development applying the traditional content analysis method. In order to comprehend the overall picture from the massive amount of LFP articles, we use a systematic and quantitative method, main path analysis (MPA), to highlight significant recent development in the field. MPA is a citation-based network analysis method which traces the most significant citation chains of a target field. The method not only hints the development trajectory but also highlights the important articles. We identify LFP main paths applying a particular approach of MPA to show the most recent research streams. Bibliometric information of 5,602 LFP articles were retrieved from the Web of Science database on September 2018. Basic analysis of the information show that the growth of LFP research continues at over 500 academic articles in each of the last five years (2013-2017). More than fifteen thousand unique researchers appear in these 5,602 articles and Chinese and U.S. scholars together produce around half of them. As regards to sources, Journal of Power Sources, Electrochimica Acta, and Journal of the Electrochemical Society are the top 3 journals that publish the largest amount of LFP articles. The main path identified is the citation chain highlighted with yellow circles in the figure. It shows that LFP research began with two Goodenough group's studies in 1997. Each of the articles on the main path is considered significant in the LFP development. For example, two early works YamadaKSK2005 [2] and GibotCLLCHTM2008 [3] show respectively that electronic conductivity can be increased through phase control and that the nanoparticle form of LiFePO₄ is beneficial to the electronic conductivity of LFP battery. Towards the end of the main path are 8 lumped-strands, which can be further categorized into two major research areas: reaction model and synthesis. The analysis suggests that most recent LFP research focuses on understanding the mechanism and establishing theoretical models for kinetic reactions as well as optimizing method to synthesize LiFePO₄ nanoparticles.

Abstract ID: 197

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Green Composites

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 ($\Gamma < -40$ 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.

Key Words: Bio-sourced composite, electromagnetic absorption, carbon particle, anechoic chamber, reflection loss.

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Abstract ID: 198

Symposium 2: Functional Composite Materials (FCM)

Invited Talk

Topics: Dielectric, Ferroelectric and Piezoelectric materials

Keywords: Carbon fibers, composites, electromagnetic absorption, anechoic chamber, dielectric properties

Carbon fibers based epoxy foam composites for electromagnetic absorption

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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 12 mm were achieved. Dielectric properties (permittivity and dielectric losses) of these materials were measured in 4 – 18 GHz frequency range. Among different filler contents, the 0.5 %wt. of 3 mm carbon fibers was the most promising sample thanks to high level of losses combined with a good homogeneity. Therefore, numerical simulations of the reflection coefficient (using electromagnetic simulation software CST) 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: 199

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Ceramic based composites

Keywords: Glass foam, electromagnetic absorption, carbon, CRT, porous structures

Carbon based 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 potentiality for high power microwave absorbing applications of these foams will be presented discussed.

Key Words: Glass foam, electromagnetic absorption, carbon

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Abstract ID: 200

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Biodetection

Keywords: Amplification effect of Nanoparticle, Detection of CRP (C reactive protein)

Au nanoparticles-enhanced optical sensor for CRP sandwich detection

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Ultra-sensitive and rapid detection of the biosensor is of great significance and urgent demand in drug detection, environmental safety, food hygiene and medical diagnosis. The surface plasmon resonance (SPR) biosensors are advanced optical label-free technology. This method is based on the detection the changes of refractive index by the capture of target analyte on the gold film surface by attached biomolecular recognition elements, and this has been used in medical diagnostics, environmental protection. The SPR biosensor has many advantages, such as anti-electromagnetic interference, high sensitivity, no fluorescence labeling, and real-time. Yet Conventional SPR is difficult to detect small molecules directly and the sensitivities are not enough to ultra-low concentration substances. Some high refractive index particles and interacting biomolecule were introduced for amplification the signal. In this study, a three dimensional nanostructure was formed in the SPR immune sandwich reaction with the Au composite nanoparticles on the surface of the SPR chip. In the SPR mode, the energy of the plasma field is strongly confined to the surface of the metal structure. The coupling between the propagating plasma and the local plasma forms a remarkable enhancement of the three-dimensional dynamic plasma field of the sandwich layer. This field is fully overlapped with the target molecules, interacting, producing the local light field of the anti-interference specific signal, and realizing the ultra-high magnification signal and fast enrichment of the optical nonlinearity. In this study, a series of concentrations of CRP (C reactive protein) were used for pattern detection, and the spectral shift signals caused by capture antibody and capture antibody-AuNPs were compared and analysed.

Thursday, 22/Aug/2019 10:30am - 10:42am

Abstract ID: 201 / FCM-2: 13

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Composites materials for Defence Technology

Keywords: 3D warp interlock p-aramid fabrics, Ballistic performance, Soft body armour, High-performance fibre

Three-dimensional (3D) warp interlock p-aramid fabrics for the development of seamless female soft body armour with better flexibility and ballistic impact performance

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Soft body armour panels were mostly produced from 2D woven, non-woven and unidirectional fabrics using different laminating methods. Recently, using three dimensional (3D) warp interlock fabrics with appropriate structure becomes a promising ballistic material for the development of seamless female soft body armour to deliver not only better ballistic protection but also better comfort and fits. This paper presents ballistic performances and energy absorption capabilities of a 3D orthogonal layer to layer (O-L) warp interlock p-aramid fabrics made of 930dTex high-performance aramid fibre (Twaron®). The fabric has been designed and manufactured on a semi-automatic loom in GEMTEX laboratory. For comparison, commercially available 2D plain weaved fabric (Twaron CT-709) made of a similar type of Twaron p-aramid fibre has been used. Each layer in the panel did not stitch together but the target panel was moulded at pre-defined two points using a newly adapted bust-shape forming bench to resemble frontal female body shape. The ballistic tests were performed according to NIJ standard-0101.06 Level-III A. The trauma indentation was used to determine energy absorption capability of different panel targets and transmit of energy to the backing material. Based on the result, the 3D warp interlock fabrics show comparable average energy absorption capabilities to counterpart 2D plain weave fabric with higher and similar number of layers. However, for a reduced number of layers, 2D plain weave fabric panel shows better ballistic performance than 3D interlock fabrics. Besides, both fabrics show less transmitted energy to the backing material at the flat target shots compared to the deformed target area. Moreover, the 3D warp interlock fabric shows better mouldability, without wrinkle formation while shaping the intended panel target, as compared to 2D plain weave fabrics. The number of layers in 3D warp interlock fabric panels has also shown a significant effect on the ballistic protection performances than 2D plain fabrics.

Abstract ID: 202

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Application of Biosensors in Drug Delivery and Clinical Chemistry

Keywords: Amplification effect of Nanoparticle, Detection of CRP (C reactive protein)

Au nanoparticles-enhanced optical sensor for CRP sandwich detection

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Ultra-sensitive and rapid detection of the biosensor is of great significance and urgent demand in drug detection, environmental safety, food hygiene and medical diagnosis. The surface plasmon resonance (SPR) biosensors are advanced optical label-free technology. This method is based on the detection the changes of refractive index by the capture of target analyte on the gold film surface by attached biomolecular recognition elements, and this has been used in medical diagnostics, environmental protection. The SPR biosensor has many advantages, such as anti-electromagnetic interference, high sensitivity, no fluorescence labeling, and real-time. Yet Conventional SPR is difficult to detect small molecules directly and the sensitivities are not enough to ultra-low concentration substances. Some high refractive index particles and interacting biomolecule were introduced for amplification the signal. In this study, a three dimensional nanostructure was formed in the SPR immune sandwich reaction with the Au composite nanoparticles on the surface of the SPR chip. In the SPR mode, the energy of the plasma field is strongly confined to the surface of the metal structure. The coupling between the propagating plasma and the local plasma forms a remarkable enhancement of the three-dimensional dynamic plasma field of the sandwich layer. This field is fully overlapped with the target molecules, interacting, producing the local light field of the anti-interference specific signal, and realizing the ultra-high magnification signal and fast enrichment of the optical nonlinearity. In this study, a series of concentrations of CRP (C reactive protein) were used for pattern detection, and the spectral shift signals caused by capture antibody and capture antibody-AuNPs were compared and analysed.

Abstract ID: 203

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Solar Cells

Keywords: ab initio, Wien2K, FP-LAPW, Chalcopyrite, physical properties.

**Prediction for optoelectronics properties of chalcopyrite's II-IV-V2 via mBJ approach:
application in thin films solar cells**

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In this research work, we investigate the structural, electronic and the linear optical properties of chalcopyrite compounds based on II-IV-V2 using an ab initio method to design new ultra thin-films solar cells with optimized performances. The computational code Wien2k based on the full potential linearized augmented plane wave method (FP-LAPW) under the framework of density functional theory (DFT) is used to predict the looked-for properties. For the exchange and correlation potential (XC), we utilized the local density approximation (LDA) only for the structural parameters. The semi-local Becke-Johnson (mBJ) potential and its modified form proposed by Tran- Blaha (TB-mBJ) used for electronic and linear optical properties. The results obtained were compared with other theoretical and experimental works.

Abstract ID: 204

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: Sulphide, Microspheres, Electrode Material, Supercapacitor

Facile preparation and high capacitance performance of copper sulfide microspheres as supercapacitor electrode material

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Copper sulfide (Cu₂S) microspheres were easily prepared by reducing copper sulphate with ascorbic acid in sodium thiosulfate solution at room temperature and employed copper sulphate and sodium thiosulfate as Cu and S sources, respectively. The as-prepared Cu₂S microspheres were characterized by scanning electron microscope (SEM), transmission electron microscope (TEM), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). The electrochemical properties including cyclic voltammetry, galvanostatic charge-discharge measurements and electrochemical impedance spectroscopy were also investigated. The experimental results showed that the as-prepared Cu₂S microspheres based on the three-electrode test system exhibited a maximum specific capacitance of 444.2 F•g⁻¹, and the energy density was up to 25.4 Wh•kg⁻¹ with high power density of 4.1 kW•kg⁻¹ at the current density of 1 A•g⁻¹. Furthermore, Cu₂S microspheres also showed outstanding long-term cycling stability with more than 87 % capacitance retention over 6000 cycles due to their microspheres structure, which facilitate efficient charge transport and promote electrolyte diffusion. The Cu₂S-1:1.5 was used as a positive electrode for the fabrication of asymmetric supercapacitor along with reduced GO as the negative electrode, which delivered the high energy density up to 18.6 Wh•kg⁻¹ along with long cycling life and retains up to 89% specific capacitance after 6000 cycles. The excellent results suggest that the Cu₂S microsphere is a promising candidate as electrode material for high performance supercapacitors.

Abstract ID: 205

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: All solid-state batteries

Keywords: Keywords: NASICON-type, $\text{Li}_{1.25}\text{Hf}_{1.75}\text{Al}_{0.25}(\text{PO}_4)_3$, structural, thermal behavior, ionic conductivity properties

**Structural, Thermal Properties and Electrical Conductivity of Al Substitution
 $\text{LiHf}_2(\text{PO}_4)_3$ NASICON-type Ionic Conductor**

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Lithium ion conducting solid electrolytes, Lithium Aluminum Hafnium Phosphate $\text{Li}_{1+x}\text{Hf}_{2-x}\text{Al}_x(\text{PO}_4)_3$ ($x = 0 - 0.75$) 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 $\text{LiHf}_2(\text{PO}_4)_3$ 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 $\text{Li}_{1+x}\text{Hf}_{2-x}\text{Al}_x(\text{PO}_4)_3$. The highest AC conductivity is observable in the sample with composition $x = 0.25$ of about $2.5 \times 10^{-3} \text{ Sm}^{-1}$ with low activation energy 0.36 eV. The present studies recommend $\text{Li}_{1.25}\text{Hf}_{1.75}\text{Al}_{0.25}(\text{PO}_4)_3$ to be a future solid electrolyte material for battery applications.

Wednesday, 21/Aug/2019 6:51pm - 7:03pm

Abstract ID: 206 / FC: 15

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalysis for chemical energy transformation and storage

Keywords: Graphene-nickel interface, dipole layer, metal deposition, electrochemical reactions, energy harvesting

Graphene-nickel interface-induced dipole layer catalytic mechanism on metal deposition and electrochemical energy harvesting

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Graphene/metal nanoparticle (G/MNP) composites have been attracting more interest because of remarkably enhanced catalytic property, which is ascribed to a synergic effect from the interface of graphene and active sites. In general, reducing agents and electrodeposition methods have been employed to in-situ reduce metal ions such as Au³⁺, Pt⁴⁺, Ag⁺, and Cu²⁺ (M^{x+}) to MNPs on the graphene to form G/MNP composites.¹ In this study, graphene-coated nickel foam (GNF) is discovered unprecedentedly to have significant catalytic effect on electrodeless metal (M: Au, Pt, Ag, and Cu) deposition on the graphene without any extra reducing agent because of electron transfer from interface electric dipole layer (EDL) induced by graphene on the nickel surface. Although the EDL model is experimentally and theoretically confirmed by work function and density functional theory (DFT) calculation, it is for the first time experimentally proved in this work. The interface EDL catalytic mechanism reveals the electron communication between graphene and nickel metal, and supports the catalytic function as an “electron bump” to accelerate the electron transfer in the metal redox reaction. In addition, the concomitant phenomenon of simultaneous formation of Ni(OH)₂ nanosheets is also elucidated. Ni(OH)₂-wrapped Ag hybrid developed on the GNF (Ag@Ni(OH)₂-GNF) is found to serve as an efficient binder-free electrochemical sensor because of its unique structure. In addition, Pt deposited on the graphene foam is found to play as a novel fuel cell electrode. It is believed that the interesting EDL catalytic mechanism will contribute to more extensive and important applications in other fields such as oxygen reduction and hydrogen evolution reactions and Li ion battery.

Thursday, 22/Aug/2019 2:51pm - 3:03pm

Abstract ID: 207 / FLNM-3: 5

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

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

Keywords: Charge-transfer salts, Electrocrystallization, Nanowire, Chemical Sensor, Nanomanufacturing

Chemical Sensor Fabrication by Direct Deposition of Organic Nanowires

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Nanowires are widely recognized as the next generation building block for ultrasensitive and ultrafast chemical detection. Despite the research progress very few nanowire sensors have reached the market due to their manufacturing complexity and high costs. We are exploring a one-step electrocrystallization method to deposit nanowires from a solution droplet at room temperature directly on electronic substrates. The nanowires are synthesized by a seed-mediated electrocrystallization mechanism. The nanoparticle-mediated electrocrystallization process was studied by cyclic voltammetry, atomic force microscopy, and field-emission scanning electron microscopy. We investigated two types of organic conductors and semiconductors, tetrathiafulvalene charge-transfer salts (TTF) and partially oxidized tetracyanoplatinate Krogmann salts (TCP), as nanowire sensors. TTF and TCP crystals grown on nanoparticle seeds displayed a confined geometry in the form of nanorods. The width of the nanorods is proportional to the diameter of the nanoparticle seed. The nanoconfinement effect is attributed to the local curvature of the nanoparticle seed that limits the width of the crystals. TTF and TCP nanowires were deposited on metallic lithographic patterns, using the pattern itself to control the deposition. The deposited nanowire interconnects are used as sensing elements for impedance-based gas sensing. The nanowire assembly shows sensitivity, selectivity, and durability suitable for the detection of chemicals such as ammonia and simulants of explosives. Our work contributes fundamental knowledge towards the scalable manufacturing of nanowire chemical sensors.

Key Words: Charge-transfer salts, Nanowire, Chemical Sensor

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Abstract ID: 208

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Polymeric composites

Keywords: Carbon nanotubes, Polymer nanocomposites, Liquid crystals, Desalination

Aligned carbon nanotube-polymer nanocomposite membranes via liquid crystalline templating for desalination and decontamination

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The use of nanotechnology to re-design osmosis membranes is an emerging technology with reduced energy consumption. In particular, single-walled carbon nanotubes show great promise for seawater desalination because of super-high flow rate of water inside nanotubes. This potential is, however, severely limited by the current inability to achieve large-scale aligned nanotube based membranes. Here we report on a liquid crystal templating methodology to prepare aligned nanotube-polymer nanocomposite membranes for desalination. The surfactant monomers with various alkyl chains of nonpolar tails form ordered liquid crystal mesophases in aqueous medium with hexagonal packing of cylindrical micelles in which nanotubes are incorporated. Under appropriate shear flow, aligned liquid crystal-nanotube mixtures are obtained. After photopolymerization, shear-induced alignment is retained in the resulting solid polymer nanocomposites. Membranes based on aligned nanotube-polymer composites are fabricated and desalination performance in terms of ion rejection, chemical separation, and water conductivity are evaluated. Our work provides promising cost-effective solution routes for the fabrication of the ordered nanotube-polymer composite membranes for seawater desalination and decontamination.

Abstract ID: 209

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Theoretical/Modelling/Computer Simulations Of Functional Materials

Keywords: Nanofluid, Functional materials, Thermophoretic diffusion, Viscous dissipation

MHD Nanofluid Heat Transfer between Parallel Plates with Thermophoretic Diffusion and Viscous Dissipation

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Unsteady MHD nanofluid flow with buoyancy driven heat transfer between two parallel plates is studied. The governing boundary layer equations are based on continuum conservation equations for nanofluids. The influence of the magnetic field is perpendicular to the flow directions applied to the lower plate which are separated by a fixed distance. The process of suction/blowing and squeezing are observed with the height variations. Solutions for velocity and temperature characteristics are obtained for two different nanofluids taking ethylene glycol as the base fluid with zirconia and silica as nanoparticles. The effects of governing parameters such as Hartmann number, thermal Grashof number, Thermophoretic diffusion, Suction/Blowing and Squeezed on dimensionless velocity and temperature profiles are computed by employing the Runge - Kutta method in MATLAB.

Nanofluids that form an important class of functional materials are nanometer sized particles suspended in the base fluid. These nano sized particles are usually metals, oxides, carbides or carbon tubes while ethylene glycol, oil and water are taken as base fluids. To measure and enhance the thermal conductivity of fluids, nanofluids are explored. Choi [1] measured the thermal conductivity of different fluids and obtained their enhancement by adding nanoparticles. Xuan [2] computed fluid flow and heat transfer features for nanofluids. Analytical investigations of nanofluid flow and heat intensification coefficients between two parallel plates are obtained by Sheikholeslami [3]. The study of unsteady nanofluids flow and heat intensification over rotating / stationary disks for different geometries under the effects of the magnetic field along with the impact of variable viscosity and fluctuating heated plate are exhaustively examined and captured by Ram et al. [4]. Lu et al. [5] explored the application of parallel geometry to study rectangular heat pipe radiator for cooling IGBT modules.

Abstract ID: 210

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Composite structural materials

Keywords: modulus of elasticity, HEAS, eutectic, borides, carbides, pseudopotential

Temperature dependence of the modulus of elasticity of materials

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In studying the physical properties of materials at high temperatures, the determining factor is the energy of the interatomic bond and the melting point temperature. To calculate the mechanical characteristics at high temperatures, the quasi-harmonic approximation model developed by the authors is used.

Strength characteristics of metals, high-entropy metal alloys (HEAS), borides, carbides, and LaB₆ – MeB₂ eutectic systems under extreme conditions (high temperature and deformation) were calculated using the a priori pseudopotential method.

In the case of composites, when calculating the modulus of elasticity, the "modified rule of mixtures" developed by the authors is used to evaluate the effect of the interface.

As a result, an analytical formula was obtained that describes the temperature dependence of the relative value of the elastic modulus for crystalline materials. For metals, there is experimental evidence of the temperature dependence of the elastic moduli.

As a result, an analytical formula is obtained describing the temperature dependence of the relative modulus of elasticity for crystalline materials. For metals, also there is an experimental confirmation of the temperature dependence of the elastic moduli.

With the help of the obtained universal relation, it becomes possible to estimate the modulus of elasticity of crystals at any temperature, if its value at zero temperature and melting temperature is known.

Abstract ID: 211**Symposium 3: Functional Catalysis (FC)****Oral Presentation**

Topics: Biomimetic catalysis

Keywords: amphiphilic polymers, nanoreactors, energy

Controlling Thermodynamics and Kinetics at the Nanoscale – Biomimicking using Functional Materials

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The use of biomimicry has become a very important and essential part of sustainable energy production. However, biological reactive systems such as proteins are optimized for maximum efficiency within narrow environmental conditions such as temperature, pH, etc. In order to develop robust systems that are stable and efficient under a very wide range of environmental conditions, we have designed nanoreactors that use the physical properties of biosystems based on functional materials. The most important factor influencing the efficiency in biological nanoreactors is the combination of (1) the effect of confinement inside the reactors and (2) a catalyst used to improve the kinetics of the reaction occurring within the nanocavity. The nanoreactor that we have developed uses a self-assembled polymeric template with alternating hydrophilic and hydrophobic cavity [1]. The confinement within the nanoreactor, which controls the thermodynamics, is linked to alternating hydrophobic and hydrophilic cavities with a size of 2-3nm [2]. The active center of the nanoreactor is obtained by an in-situ reduction of AuCl producing monoatomically thin layers of gold. The gold monolayer showed a very high catalytic efficiency compared to Pt nanocatalyst obtained using the same conditions [3]. The nanoreactor is stable in aqueous environment under various pH (pH2-12) and broad temperatures range 4oC to 80oC. The synthesis, characterization and a complete kinetic study of a model reaction will be presented.

Key Words: amphiphilic polymers, nanoreactors, energy

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Abstract ID: 212**Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)****Oral Presentation**

Topics: Computational modeling and simulation of low dimensional, nano and 2D materials

Keywords: Phthalocyanine, one-dimensional, magnetic, optical

Magnetic and optical properties of metal-phthalocyanines: A low-dimensional organic semiconductors

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Organic semiconductors based on phthalocyanine molecules have been proven to be a promising material candidate in nano-magnetism [1, 2], optical devices [3], and quantum information processing [4]. These organic materials are formed by the one-dimensional molecular chains. In this presentation, I will first discuss recent theoretical and experimental work on the photon-detector devices consisting of copper-phthalocyanines with fast optical response [1]. In addition, I will discuss the magnetic properties of transition-metal phthalocyanines, including copper-, cobalt, chromium-, and lithium-phthalocyanines [5, 6, 7, 8]. We have demonstrated theoretically and experimentally that cobalt-phthalocyanines have a magnetic transition temperature higher than the boiling point of nitrogen [5, 6], which is very promising for magnetic information storage and spintronics. Theoretically we have also shown that there is a huge potential in magnetism for lithium-phthalocyanines [8], in which a large exchange interaction arises from the p-orbitals of carbon/nitrogen atoms. The strong anti-ferromagnetic interactions in these molecular chains can be explored for spintronics based on anti-ferromagnetism. By combining copper- and cobalt-phthalocyanines, we can form ferromagnetic chains artificially, leading to organic magnetic meta-materials [9]. Using optical excitations and inter-system crossing, optical control of spin-spin interaction can be realized in molecules, which has a great potential in spintronics and optoelectronics [10].

Key Words: Phthalocyanine, one-dimensional, magnetic, optical

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Thursday, 22/Aug/2019 2:24pm - 2:36pm

Abstract ID: 213 / FESC-2: 3

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: graphene, bipolar electrochemistry, energy storage

Electrochemical Characterization of Bipolar Electrochemically Exfoliated Graphene

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Graphene has attracted a considerable interest in different fields such as energy storage devices, gas sensors, and cancer detection due to its unique properties like high surface area, broad electrochemical window, high electrical and thermal conductivity, high charge carrier mobility, and high transparency. However, the production of graphene-based devices still suffers from various challenges. First, the quality of the graphene production is still poor. Commercial available graphenes contain various microplatelets with large distribution of size and numbers of layers indicating most of them are not optimal for practical applications. Second, harsh chemicals used in wet chemical exfoliation of graphene process are costly and not environmental friendly. Third, both production and integration of graphene for device fabrication (including CVD approach) are not only time consuming, complicated, and expensive, but also hard to control the quality of material assembly, surface condition, and device performance. Therefore, better methods for graphene production is urgently needed. In this work, we designed a one-step process using the bipolar electrochemistry concept to produce and deposit high quality graphene layers directly on metallic substrates from highly pure graphite rod. This process combines material production and device fabrication in one simple and controllable step. It is confirmed by various materials characterization approaches that both graphene oxide and reduced graphene oxide can be selectively assembled onto the current collectors. High electrochemical performance of the products was obtained by cyclic voltammetry, electrochemical impedance spectroscopy, and galvanostatic charge discharge tests. Detailed results and discussion will be presented in conference.

Thursday, 22/Aug/2019 11:36am - 11:48am

Abstract ID: 214 / FTF: 4

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Optical, electrical and magnetic properties of thin films

Keywords: photonic crystals, wettability, self-assembly

Superwettability of Colloidal Photonic Crystals

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Photonic crystals (PCs) demonstrate important applications in new optical devices owing to special property of light regulation[1]. This paper presents a series of functional PCs based on its special wettability. As-prepared metal-organic (Pb(NO₃)-COOH) PCs can achieve irreversible changes in color/morphology during the electrowetting process, developing a novel and simple water-lithography approach for the creation of the PC pattern[2]. The close-cell carbon dots inverse opals, which prepared from organosilane-polymerized carbon dots and low temperature process, show unique lyophilic but nonwettability[3]. In addition, the special optical properties of the carbon dots endow the sample with tricolor-fluorescence, fluorescence enhancement and modulated optical limiting performance, making it well used in anti-fake pattern[4]. A novel humidity-induced actuator is prepared by the gradient wettability of polyionic liquid inverse opals[5]. Furthermore, Janus PC films can be obtained by asymmetric filling. The directional actuation and thermal shape memory function of PVDF PCs have been realized[6]. A colloidal microarray with optical waveguide behavior is obtained by using a superwettability assembly of fluorescent dye particles[7]. These works are of great significance for the preparation of multi-functional PC materials and new optical devices.

Abstract ID: 215**Symposium 6: Functional Thin Films (FTF)****Poster Presentation**

Topics: Thin films for optoelectronics, nanoelectronics and spintronics

Keywords: Sb₂S₃, annealing, bandgap, dopants, absorbers.

Morphological and optical properties of chemically deposited magnesium doped-antimony sulphide thin films for use in optoelectronic applications

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Thin films of antimony sulphide (Sb₂S₃) were grown using the chemical bath deposition technique. The films were doped using different concentration of the dopants (magnesium impurities (0.1 M – 0.3 M)). This films were annealed in a furnace at different temperatures of 100 oC , 200 oC and 300 oC, and time for 1 hour respectively. The effect of the different concentrations of the dopants and annealing treatments on the films were investigated with emphasis on the morphology, and optical properties such as transmittance, absorbance, reflectance, optical absorption coefficient, energy bandgap, refractive index, and the dielectric constants. The electrical resistivities of the layers were also deduced from the optical measurements. The results indicate that the different annealing temperatures and dopants concentrations influenced the morphology, film thicknesses, optical and electrical properties significantly. The transmittance of the films were all > 40% in the UV-VIS region. A shift in the cut-off wavelength was also observed after annealing. The energy bandgap was found to be direct in both the as-grown and heat treated layers. The energy band gap was observed to be in the range of 1.25 eV to 1.72 eV, and the dopants induced a Burstein-Moss shift in the energy band gap of the as-grown films within some range of the concentration of the dopants. In the annealed case the energy band gap was observed to be in the range of 1.15eV to 1.35eV, and the annealing treatments shifted the energy band gap toward lower photon energies (longer wavelengths) for dopants concentration of 0.1 M, and changed otherwise for higher concentrations of the Mg²⁺ ions . This is due to quantum size effect induced by the annealing treatments within that regime. The extinction coefficient (k) decreased uniformly with the increase of the Mg²⁺ ions with values from 0.02 to 0.18. The annealed layers had values between 0.001 and 0.04 and decreased in the reverse direction. The values of the energy bandgap are within the range suitable for use of the layers in optoelectronic devices including absorbers in hetero-junction solar cell devices.

Keywords: Sb₂S₃, annealing, bandgap, dopants, absorbers.

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Thursday, 22/Aug/2019 12:36pm - 12:48pm

Abstract ID: 216 / FCM-3: 9

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Composites in Innovative Applications

Keywords: Lost circulation materials, Core-shell structure, Composite, Shape memory alloy, Self-cementation material

Preparation and study on core-shell structure composite lost circulation material based on shape memory alloy in drilling engineering

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Lost circulation is defined as the loss of drilling fluids to formation void during drilling process, which is one of the major issues that leads to increase of costs and the nonproductive time of the operation. Lost circulation in fractured formations is the most common form. The addition of conventional granular, flakes and fibrous lost circulation materials (LCMs) with combination is the most common way to control loss circulation with the effect of bridging and filling in fractures. However, the conventional lost-circulation treatments are often based on trial and error methods without any practical technique to properly diagnose and characterize the loss zone. A core-shell structure composite lost circulation material (CS-LCM) containing shape memory alloy (SMA) and self-cementation material as core, and cement as shell was prepared. Shape memory alloy was prepared as a spring-shape initially. Self-cementation material was filled into the spring. Then the agglomerant was sprayed on the surface of the spring and treated with granulating in the cement by rolling in disc granulator.

The particle size of the CS-LCM is 5-20mm. It can be combined with other conventional LCMs to cure loss. The sealing ability was evaluated by plugging apparatus with long fracture slot. When reaching phase transition temperature (60-90 °C), the shape memory alloy changed from spring-shape into line-shape, which resulted in cement shell broken. The elongated SMA overlaps and bridges in fracture to form a network structure. The cement and other LCMs can fill the void spaces within the network structure. The hydrate products of self-cementation material can fill between particles, then cement the SMA, LCMs and the fracture wall together. It can improve the strength and retention capability of the seal. It is possible to design a smart LCM based on shape memory alloy which does not depend on the opening width of the formation fracture. This study offers a promising route to cure the severe loss in fractured formations.

Thursday, 22/Aug/2019 2:51pm - 3:03pm

Abstract ID: 217 / FCM-4: 5

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Experimental methods for Composite materials

Keywords: Fatigue, Fracture, Elevated Temperature, Crack, Nanocomposite

Fatigue Responses of Ti/APC-2 Nanocomposite Laminates with Inclined Cracks at Elevated Temperature Part I: Experiments

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The mechanical properties and fatigue responses of Ti/APC-2 hybrid neat and nanocomposite laminates with inclined single-edged cracks due to tensile and cyclic tests at elevated temperature were investigated. Two types of composite laminates (Ti/(0/90)_s/Ti) were fabricated such as with and without (w/wo) nanoparticles SiO₂ of optimal 1 wt.%.

The geometry and dimensions of specimens were $L \times W \times t = 210 \times 25 \times 1.55 \text{ mm}^3$. The cracks were of constant length 3mm and width 0.3mm. The inclined angles were 0°, 45° and 60°. Both the tensile and cyclic tests were conducted at elevated temperatures 25 °C (RT), 100 °C and 150 °C. From the tensile tests we obtained the loads vs. displacement curves for both types of laminates, with varied inclinations at elevated temperatures. Next, we received the applied load vs. cycles curves for the laminates with inclined cracks at high temperature due to cyclic tests. According to the experimental data of both tensile and cyclic tests the mechanical properties, such as strength, stiffness and life, were decreased as temperature increasing. The greater the inclined angles were, the greater the strength and stiffness were. Similarly, the fatigue life was in the same trend. However, the effect of inclined angle on mechanical properties was more significant than those of temperature. The mechanical properties of nanocomposite laminates were higher than those of neat composite laminates, but not significant. The main reason was the enhancement of spreading nanoparticle silica on the laminate interfaces did not strongly lower the stress intensity at the crack tip locally.

In life analysis we used the fracture toughness and J-integral. The Paris law was modified to predict the crack growth rate and residual life of cracked composite laminates. In the consideration of bridging effect, enhancement by nanoparticles and the failure mechanism at elevated temperature the effective stress intensity factor range were obtained. Comparing with experimental data we found that the predicted results were well accepted with errors.

Wednesday, 21/Aug/2019 6:48pm - 7:00pm

Abstract ID: 218 / FCM: 15

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Applications of Composites

Keywords: Bisphenol F, Zinc oxide reduced graphene nanocomposite, Modified Carbon paste electrode, Drop cast deposition, Endocrine disruptor.

ZnO/G nano composite and CTAB surface modified carbon paste electrode architecture as an electrochemical sensor for the detection of endocrine disruptor Bisphenol F

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Due to the enforcement of regulatory restrictions to prevent risk to human health from Bisphenol A (BPA), its structural analogue Bisphenol F (BPF) has been introduced into the market as an alternative. But however recent studies describe BPF as an effectual endocrine disruptor. Hence, there is an indispensable need for research concerning BPF human and environmental exposure level. In addition to that the surveys conducted by USA, Canada and China ascertain the predominant BPF leaching in food items [1-3]. In this work, we have elicited the development of an economical electrochemical sensor, to quantify and investigate in detail the electrochemical behavior of BPF using carbon paste electrode modified with zinc oxide reduced graphene nanocomposite (ZnO/G) and cetyltrimethyl -ammonium bromide (CTAB). The ZnO/G was synthesized using Hummers method and characterized by spectroscopic techniques. ZnO/G is considered as an excellent functional material due to their combined individual properties which offer abundant active sites for reactions to occur. CTAB monolayer exhibits additional synergetic interactions with ZnO/G layer; this effect promotes higher sensitivity and selectivity towards target BPF molecules. Under optimal conditions, ZnO/G/CTAB/MCPE offered ultra sensitivity for BPF recognition by Differential Pulse Voltammetry, with a detection limit of 0.06 μM . Lowering of activation energy for electro-oxidation of BPF and absence of peak for interfering molecule Ascorbic acid makes it an unique sensor for the detection of BPF with significant analytical advantage over other sensors reported in literature. Versatility of the electrode was demonstrated by applying it to real time analysis of human body fluids, canned beverage and different water samples fortified with BPF. The satisfactory recoveries obtained, consequently authenticates the practicality of the proposed sensor.

Key Words: Bisphenol F, Zinc oxide reduced graphene nanocomposite, Modified Carbon paste electrode, Drop cast deposition, Endocrine disruptor.

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Abstract ID: 220

Symposium 2: Functional Composite Materials (FCM)

Invited Talk

Topics: Ceramic based composites

Keywords: BaTi₂O₅; hydrothermal method; Nanostructures; Monoclinic phase; Dielectric properties.

The Optimum Conditions in Preparation of BaTi₂O₅ Nanostructure by Hydrothermal Method

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The preparation of BaTi₂O₅ as a dielectric ceramic compound had been done through the hydrothermal process depending on different conditions such as, pH-value, the reaction time, the temperature and pressure. The prepared powders were examined by X-ray diffraction (XRD). It was found the presence of monoclinic phase of BaTi₂O₅ with (space group C2/m), and unit-cell parameters of (a=16.6381, b=3.555, c=9.3406 Å), ($\beta=107.47^\circ$, $\alpha=\gamma=90^\circ$), and the volume $V=527 \text{ \AA}^3$. The predominant phase was a monoclinic phase, but difference in the lattice constants. The surface morphology was demonstrated by Scanning Electron Microscopy (SEM). It was exhibited the grains like a spherical and elliptical shapes with high homogeneity. The shapes of nanostructure were analyzed by Transmission Electron Microscopy (TEM). It was found that the appearance of nanostructures like the nanoparticles, Nano rode and Nano sheet. The nanoparticles was in the range of (9-31 nm), Nano rode in size of (36.7 nm), and Nano sheet in size of (971.15 nm). The dielectric measurements were done by using LCR meter with different frequencies (10, 50 and 100 KHz). It was clear that the Curie temperature have a high value up to (485°C).

Abstract ID: 221

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Computational modeling and simulation of low dimensional, nano and 2D materials

Keywords: Nanowire, gold nanocluster complexes, nanoelectronics

Optical and charge transport properties of gold-nanocluster complexes: single-molecule nanowires

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Relativistic time-dependent density functional theory calculations were performed to obtain the absorption spectra of gold-cluster complexes (cluster-molecule-cluster) Au₄-S-C_nH_{2n}-S'-Au₄' (n=2-5). The charge transfer (CT) rate constants were also calculated within Marcus theory. The electronic, optical and CT properties were analyzed as a function of the system size (n). The range-separated exchange-correlation functional CAMB3LYP was used to properly predict charge transfer excitations. Overall the absorption spectrum remains quite similar with size for those gold-cluster complexes whose structure and metal-molecule bonding remains similar too. This is the case for complexes with n=2,4,5, for which the absorption spectrum has its main peak at 320nm with a shoulder at 430nm, and a secondary peak at 580nm. However, the gold-cluster complex with n=3, that has a different structure and bonding at the metal-molecule interface, shows an extra peak in the infrared range (1194nm) and excitations of CT character. The CT rate constant was calculated for the complexes n=2-3 resulting a value similar to those reported in solar cells (>10¹¹s⁻¹).

Abstract ID: 222

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

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

Keywords: Organic Photovoltaics, charge transfer, DFT

Van der Waals effects on the Optical and Charge Transfer Properties in Organic Photovoltaics

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We have recently reported that dispersion forces can have drastic effects on the structure and charge separation in organic photovoltaics [1]. In this work we show the effects of van der Waals interactions on the structure and the UV-Vis absorption spectrum of series of dimer complexes formed by the polymer P3HT and the fullerene derivative PCBM. Time-dependent density functional theory calculations demonstrate that the experimentally observed blue-shift of the absorption maximum in the active layer of P3HT/PCBM OPV cells with respect to the absorption of pure P3HT results mainly from distortions in P3HT due to van der Waals interactions between donor and acceptor fragments. Reduced absorption in the red region of the UV-Vis spectrum results from distortions of P3HT and small charge transfer between P3HT and PCBM. These results are in qualitative agreement with experiments and recent theoretical results on the corresponding solid-state films. Charge transfer rate constants were also computed within Marcus theory for dimers P/PCBM for some semiconductor polymers (P) used in high efficient OPVs [2].

Key Words: Organic Photovoltaics, charge transfer, DFT

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Abstract ID: 223

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Bio-inorganic nanomaterials

Keywords: atomically precise nanomaterials

Atomically Precise Hybrid Nanoparticles with Multivalent Capabilities

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Unlike proteins and small-molecules, hybrid nanoparticle assemblies are never atomically precise and therefore have non-uniform composition and size. This fundamentally limits the researcher's ability to precisely engineer recognition and binding properties of these assemblies. This is especially true of a large class of hybrid noble metal nanoparticles including gold-based systems (AuNPs). Weak metal-ligand interactions contribute to a statistical distribution of defects and positional uncertainty of ligands around the metal core, limiting their molecular precision. Consequently, inherent polydispersity features of hybrid nanoparticles leads to their diminished selectivity when they are designed to target and bind biomacromolecules. Furthermore, under relatively benign conditions, weak metal-ligand interactions in the hybrid nanoparticles can result in scrambling events and ultimately degradation. Therefore, the status quo in the field largely centers on our inability to rationally address structure-function properties of hybrid nanomaterials.

Our work can be characterized as a “nanoparticle total synthesis”, where we are utilizing a bottom-up approach for the synthesis of large hybrid molecules using atomically precise 3D inorganic clusters as rigid templates. Specifically, we developed a new strategy for building robust, atomically precise hybrid nanomolecules using air-stable inorganic clusters densely decorated with perfluoroaromatic functional groups. This strategy is very appealing given its similarity to the synthesis of AuNPs; however, in this case, the resulting structures maintain full atomic precision and exhibit dramatically improved stability due to the full covalency of the resulting systems. In my presentation, I will show how this strategy can be used for facile attachment of receptor building blocks and positioning these in three-dimensions with an atomic precision. I will furthermore highlight our recent effort in improving the attachment chemistry to render the assembly of these structures more facile.

Ultimately, our work should help to promote a thorough understanding of the design rules governing interactions between hybrid nanomaterials and biomolecules and elucidate the dominant factors that enhance specific inhibition of complex biomolecular targets. For the first time, combining elements of inorganic cluster chemistry, chemical biology and materials science we will enable researchers to create well-defined programmable hybrid nanosystems with unique capabilities for binding and sensing complex biomolecules.

Abstract ID: 224

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Bio-inspired design of composites

Keywords: Antifreeze proteins, ice formation

Bioinspired Materials for Controlling Ice Nucleation, Growth, and Recrystallization

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Ice formation, mainly consisting of ice nucleation, ice growth, and ice recrystallization, is ubiquitous and crucial in wide-ranging fields from cryobiology to atmospheric physics.¹⁻⁴ Despite active research for more than a century, the mechanism of ice formation is still far from satisfactory. Meanwhile, nature has unique ways of controlling ice formation and can provide resourceful avenues to unravel the mechanism of ice formation.⁵⁻⁶ For instance, antifreeze proteins (AFPs) protect living organisms from freezing damage via controlling ice formation, for example, tuning ice nucleation, shaping ice crystals, and inhibiting ice growth and recrystallization. In addition, AFP mimics can have applications in cryopreservation of cells, tissues, and organs, food storage, and anti-icing materials. Considering practical applications and conditions, a correlation between the polyelectrolyte surface molecular structure and various AFP-inspired materials with different capabilities in controlling ice formation has been established experimentally and theoretically. We also design application-oriented materials in order to meet the needs of anti-icing and cryopreservation.

Abstract ID: 225

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biomimetic materials

Keywords: Living Functional Materials, Synthetic Biology, Bacterial Biofilms, Self-assembly

Engineering Living Functional Materials with Synthetic Biology

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Bacterial biofilms are multifunctional and environmentally responsive assemblies of living and non-living components. We introduce here a living functional materials platform based on engineered bacterial biofilms by leveraging the power of synthetic biology. We demonstrate that such programmable bacterial biofilms enable a radically different paradigm of materials synthesis and performance as well as new opportunities for constructing smart multifunctional materials and nanotechnologies. Specific examples include: (1) dynamic assembly of inorganic nano-objects with precise spatiotemporal control, (2) recyclable organic/inorganic hybrid catalysis system for artificial photosynthesis, and (3) living cellular glues for autonomous repairs. Notably, the engineered biofilms have the viscoelastic behaviors of hydrogels and can be precisely fabricated into microstructures having a diversity of three-dimensional (3D) shapes using 3D printing and microencapsulation techniques. This new tunable platform offers previously unattainable properties for a variety of living functional materials having applications in biomaterials, biotechnology, bioenergy and biomedicine.

Key words: Living Functional Materials, Bacterials biofilms, Synthetic Biology

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Abstract ID: 226

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biomimetic materials

Keywords: spider silk, functional materials, protein structure, fiber spinning

Spider Silks: A Source of Inspiration towards Revolutionary Functional Materials

Jinlian HU, Harun Venkatesan, Jianming Chen, Yuanzhang Jiang, Lin GU

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Spider silks is the collective name for a family of seven different fibers from one spider for web forming, its living and reproduction. They are spun by spinnerets in its abdomen with protein dope secreted from its individual spider glands. These seven fibers serve different functions in the web construction for the whole life of the spider. Each fiber has its own gene sequence for amino-acid repeating motifs and its termini structure, which endows the diversity of protein structures with a wide array of extraordinary properties and purposeful uses. For example, dragline silk is responsible for the formation of web frame with extraordinary strength, modulus and toughness while eggcase fiber is used for the protection of the moth within the case with a flat stress-strain curve and spiral thread is for capturing its preys. With understanding of working mechanisms and natural laws for silk hierarchical structure formation and their functions as well as technological advancements, spider silks will become a very rich source of inspiration for making various revolutionary materials in artificial muscles, high-performance space materials, military protective clothing, drugs, medical devices, optics, electronics, regenerative medicine and composites applications. This paper will introduce the state-of-the-art technologies from chemistry, nanomaterials to genetic engineering leading to this resilient and sustainable future of revolutionary functional materials.

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Abstract ID: 227

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Theory of Structure, Surface and Interface of thin films

Keywords: Thin film, metal oxides, Non Fermi liquid behavior, Perovskite Nikalates, Metal to Insulator transition

Tuning non-Fermi liquid behavior by Oxygen variation and epitaxial strain in PrNiO_{3-δ} thin films

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Tuning non-Fermi liquid behavior by

Oxygen variation and epitaxial strain in PrNiO_{3-δ} thin films

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Abstract

The observations of non-Fermi liquid (NFL) state, a feature associated with quantum criticality, in perovskite thin films of RNiO₃ (R=Rare earth ion) recently have caused upsurge in the research in this direction. The parameters like strain and pressure are known to influence the NFL behavior in RNiO₃ system. To understand the effects of oxygen variation in combination of different strain, three sets of PrNiO_{3-δ} thin films (S1, S2 and S3) were deposited on (001) oriented single-crystal wafers of, respectively, SrTiO₃, [(LaAlO₃)_{0.3}(Sr₂Al-Ta₆)_{0.7}] and LaAlO₃. Two sets of films, S1 and S2, have tensile strain whereas the films in S3 show compressive strain. For each set, two thin films of fixed thickness (5 nm) were deposited; one film was post-annealed in oxygen partial pressure for sufficient oxygen stoichiometry and another film was made oxygen deficient. These films show NFL behavior in the metallic state. Moreover, the fitting parameters to power law equation show a systematic tuning of NFL fitting parameters because of variations in strain and oxygen content. Our results show that, not only the strain, but also the oxygen content of the films is another crucial parameter in tuning the NFL behavior and electronic properties of RNiO₃ films.

Key Words: perovskite, thin films, non-Fermi liquid

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Wednesday, 21/Aug/2019 5:36pm - 5:48pm

Abstract ID: 228 / FCM: 9

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: Stimuli-Responsive, Protective Membranes, Carbon Nanotubes

Stimuli-Responsive Carbon Nanotube Membranes for Chemical Warfare Protection

Chiatai Chen¹, Yifan Li², Eric Meshot¹, Ngoc Bui¹, Rong Zhu², Myles Herbert², Sei Jin Park¹, Steven Buchsbaum¹, Melinda Jue¹, Kuang Jen Wu¹, Timothy M. Swager², Francesco Fornasiero¹

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Conventional protective garments are passive systems that sacrifice breathability to prevent exposure to harmful agents. This trade-off can lead to overheating in extended wear of protective clothing and, thus, severely hinders the duration of their active use. For personnel protection from chemical and biological (CB) agents, smart dynamic materials that exhibit a reversible, CB-triggered transition from a breathable state to a protective state are expected to be particularly effective in mitigating physiological burden because a less breathable but protective state can be actuated locally and only when needed.

To achieve adaptive protection and simultaneous thermal comfort, we have developed a chemical-threat-responsive, surface-functionalized membrane, in which vertically-aligned sub 5-nm carbon-nanotubes (CNTs) function as the only transport pathways. Before functionalization with chemical-warfare-agent responsive polymers, these membranes provide water vapor transport rates (MVTR) up to 11,000 gr/m²day, thus exceeding state-of-art breathable fabrics. Measured water-vapor permeability in 1.9-nm CNT channels is ~100 times larger than Knudsen diffusion prediction. Filtration tests with multiple analytes demonstrate that these CNT membranes provide also a high degree of protection from bio-threats by size exclusion.¹

When actuating polymers responsive to G-agents are grafted to the CNT membrane surface,^{2,3} these multifunctional membranes are able to switch from a breathable state with MVTR > 4,000 gr/m²day to a protective state with MVTR > 1,000 gr/m²day upon exposure to simulants. This transition is enabled by a threat-triggered collapse of the polymer chains, which close the CNT pore entrance to chemicals permeation. Simulant transport in the protective state is reduced by 2 orders of magnitude. The membranes can be regenerated to the open state with a simple base treatment and re-used for multiple cycles without performance loss.

Adaptive multifunctional membranes based upon this platform present exciting opportunities in many other areas including separation processes, sensing, and smart delivery.

Thursday, 22/Aug/2019 2:39pm - 2:51pm

Abstract ID: 229 / FLNM-3: 4

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nanomaterials for Energy and Environmental Applications

Keywords: Large-Area Membranes, High-Density SWNTs, Nanofiltration, Chemical Resistant

Wafer-scale nanofiltration membranes with a high density of narrow SWNT pores

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Enhanced fluid transport in single-walled carbon nanotube (SWNT) channels promises to enable major advancements in several membrane applications, from efficient water purification [1] and low-cost recovery of high-value components, to breathable and protective fabrics [2]. Furthermore, in the water treatment area, the chemical robustness of SWNTs may allow membrane regeneration with aggressive cleaning methods, which are detrimental for conventional membranes. Realization of the SWNT-membrane potential in practical applications has been hampered by the challenges in fabricating large-area membranes with a high density of open, small-diameter, SWNT pores. A high tube density is required to provide flow rates outperforming those of commercial membranes, whereas small diameters enhance both size and charge based selectivity.

To address these issues, we have developed growth recipes for vertically aligned SWNT that minimize SWNT diameter (down to <2-nm average diameter) and maximize number density (up to 2×10^{12} tubes/cm²) while simultaneously scaling up SWNT growth area (up to 4-in diameter). By filling the intertube gaps with a chemically resistant polymers and then opening the SWNT caps with dedicated etching steps, we have demonstrated SWNT membranes at 4-in scale with nitrogen and water permeances approaching 4×10^{-5} mol/m² s Pa and 250 LMH/bar, respectively, thus outperforming other large-area CNT membranes by 1-2 orders of magnitude. These membranes fully reject nm-sized dyes and particles, are compatible with aggressive cleaning methods, and show great promises in the nanofiltration area.

Abstract ID: 230

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Fundamental investigations on low-dimensional nanomaterials and their functional structures properties

Keywords: CNTs, Fast Diffusion, Ions

Fast ion diffusion in carbon nanotube pores

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Many simulations and experiments have investigated pressure-driven fluid flow in carbon nanotubes (CNTs) and demonstrated enormous transport rates through these channels. Comparatively little attention has been given so far to concentration-driven transport [1] in CNTs despite its importance, for ex., for dialysis applications. A few studies suggested or assumed bulk/hindered diffusion for small molecules through nm-wide CNTs. In contrast, other simulations have predicted self-diffusion coefficients in CNTs several times larger than in the bulk, and NMR experiments supporting these claims are beginning to emerge. These large uncertainties in the magnitude of the diffusion rates through CNTs have hampered their full exploitation in fluidic devices [2].

To obtain a precise quantification of the diffusive flow in CNTs, we have fabricated membranes with a large but known number of single-walled carbon nanotubes as fluid transport pathways. Contrary to previously employed systems, this platform enables us to minimize uncertainties in the calculation of the flow rates through a single pore. Our measurements indicate that the transport diffusivity of small ions in single-walled carbon nanotubes is about three times faster than in the bulk. These results shed further light onto the unique transport properties of graphitic channels and enable a more accurate design of CNT-based fluidic systems for a broad range of applications.

Abstract ID: 231

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: All solid-state batteries

Keywords: Solid-state batteries, Nanogenerators, Self-powered systems

Solid-State Li/Na Batteries and Self-Powered Systems

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All-solid-state batteries contain nonflammable solid electrolytes that offer high safety compared to conventional batteries with liquid electrolytes. Moreover, all-solid-state batteries can increase cycle life, energy density and reduce the requirements on packaging [1]. Triboelectric nanogenerators (TENGs) can be used to harvest various kinds of mechanical energy. However the energy harvested by TENGs cannot be directly used to provide stable power output subsequently because of the randomness of mechanical energy source and pulsed alternating current (AC) output [2]. Therefore, efficient and durable energy storage devices are highly desired to store the electrical energy harvested and converted from mechanical energy by TENGs. We developed several solid-state batteries and integrated them with TENGs. First, we demonstrated an all-solid-state Na-ion battery with safe and durable performance used for efficient storing pulsed energy harvested by the TENG. The solid-state sodium-ion battery was charged by galvanostatic mode and pulse mode with the TENG, respectively. The all-solid-state sodium-ion battery displays excellent cyclic performance up to 1000 cycles with a capacity retention of about 85% even at a high charge and discharge current density of 48 mA g⁻¹. When charged by the TENG, an energy conversion efficiency of 62.3% was demonstrated. Moreover, a garnet (Li₇La₃Zr₂O₁₂)-based hybrid solid electrolyte (HSE) membrane was designed for high performance solid-state lithium batteries. The composite HSE membrane is composed of LLZO particles and PVDF–HFP polymer matrix. The solid-state lithium battery with this HSE membrane, Li metal anode and LiFePO₄ cathode exhibits an initial reversible discharge capacity of 120 mA h g⁻¹ at a charge/discharge current density of 0.5 C at room temperature. This solid-state battery is also used to store the energy harvested by a TENG at different rotation rates. The solid state battery can efficiently store the pulsed energy, especially for output at high frequencies. The integration of TENGs with the safe and durable solid-state Li/Na batteries is potential for providing more stable power output for self-powered systems.

Abstract ID: 232

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

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

Keywords: 2D Materials, Phosphorene, Density Functional Theory, Energy Storage

Adsorption and diffusion on a phosphorene monolayer: a DFT study

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The increasing interest in future energy storage technologies has generated the urgent need for alternative rechargeable lithium, sodium, magnesium and other different ion batteries due to their high reversible capacity, high energy density and good cycle life.

In this work, a computational study of the adsorption and diffusion behavior of alkali (Li, Na and K) and alkaline earth metal (Be, Mg and Ca) atoms on a phosphorene monolayer is reported. Our calculations were performed within the framework of density functional theory using the Perdew–Burke–Ernzerhof functional and projector augmented wave potentials, as derived from the generalized gradient approximation. Our binding energy calculations for various potential adsorption sites showed that the site located above the center of a triangle formed by three surface phosphorus atoms is the most attractive to all adatoms. In addition, simulation of the diffusion of adatoms across the surface of the phosphorene monolayer showed that the diffusion is anisotropic, with K having the lowest diffusion barrier (0.02 eV along the zigzag pathway). To the best of our knowledge, this is the lowest diffusion barrier of any metal adatom on a single layer of phosphorene. While phosphorene exhibited significantly better adatom adsorption and diffusion than graphene, it also showed a reduced storage capacity compared to graphene, most probably due to the structural distortion induced by the oversaturated phosphorene surface. This finding strongly suggests that a phosphorene–graphene hybrid system could be employed as a promising high-capacity ion anode.

Thursday, 22/Aug/2019 3:39pm - 3:51pm

Abstract ID: 233 / FESC-2: 9

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Piezotronics for smart systems

Keywords: Niobate, Rod-like, Piezoelectric, Sensors, Synthesis

Synthesis of One-dimensional multi-Niobate composited and their Application of Flexible Piezoelectric Films

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In recent years, piezoelectric micro-nano devices based on piezoelectric effect have attracted much attention and have a good application prospect in sensing, wearable, biocytology, self-generating devices and integrated circuits. In this study, we proposed a synthesis of environmentally friendly perovskite-type rod-like multi-niobate method, rod-like (Li, Na, K) (Nb_{0.96}Sb_{0.04}) O₃ were synthesized by the topological melting salt reaction with rod-like K₂ (Nb_{1-x}Sb_x)₈O₂₁. The molar ratio of sodium salt, (Li, Na, K) (Nb_{0.96}Sb_{0.04}) O₃ material was synthesized at approximating its quasi-isomorphic boundary. The ink of piezoelectric rod-like (Li, Na, K) (Nb_{0.96}Sb_{0.04}) O₃ combined with PDMS (Rod-LNKNS-PDMS) was prepared. The piezoelectric films with different thickness were prepared by spin coating method. Compared with the normal (Li, Na, K) (Nb_{0.96}Sb_{0.04}) O₃ particles obtained by typical solid phase synthesis, and the electrical properties of the output voltage of the Rod-LNKNS-PDMS piezoelectric films showed about 2.5 times higher. This kind of aligned rod-like material can effectively improve the output signals, with great potential on the application of flexible piezoelectric sensors.

Abstract ID: 234

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Realization and application of nanodevices electronics, optoelectronics, photonics, energy harvesting, biological sensing, composite, and so forth

Keywords: semiconductor, two dimensional materials, Nanostructure, Photodetector

Special functional photodetectors based on low dimensional materials

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As a momentous component of information technology (IT), photoelectric sensor technology has attracted considerable attention owing to its tremendous application potentials in many domains with regard to industry, agriculture, environment and medical care. In particular, cooperated with communication technology and computer technology, versatile photodetectors with special functions provide us great abilities to understand and change the world [1,2]. Therefore, further research and development of special functional photodetectors will be of great significant both in human health and social progress.

With getting deeper insights into the interaction between light and matter at nanoscale, versatile nanostructured photodetectors with special functions such as self-powered photodetectors, binary response photodetectors, and dual-band photodetectors have been explored in our group [3-6]. These studies offer promising route for the future applications of these kind of high-performance multifunctional photodetectors, and we do hope this presentation will inspire an increasing number of researchers and engineers to join this game.

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Abstract ID: 235

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Catalyst Design, Synthesis and characterization

Keywords: titania; nanotubes; reductive annealing; doping; photocatalysts; crystal defects

Adsorption and catalytic behaviors of Fe-doped titania nanotubes treated reductively

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The Fe-doped titania nanotubes were hydrothermally synthesized using Fe-doping anatase nanopowder precursors and annealing in air and reductive atmospheres; the evolution of phase and morphology of titania nanotubes in hydrothermal synthesis were studied; the microstructure and physicochemical properties of the nanotubes were investigated. The nanotubes had a diameter of 5 nm and a length of 100 nm and an (101) orientation. The hydrothermal reaction stimulated the transformation of amorphous to $\text{Na}_2\text{Ti}_2\text{Ti}_6\text{O}_{16}$ flakes; the acid-washing promoted the transition of $\text{Na}_2\text{Ti}_2\text{Ti}_6\text{O}_{16}$ flakes to $\text{H}_2\text{Ti}_4\text{O}_9 \cdot \text{H}_2\text{O}$ nanotubes and the calcination improved $\text{H}_2\text{Ti}_4\text{O}_9 \cdot \text{H}_2\text{O}$ nanotubes transforming into titania nanotubes. The reductive pre-annealing yielded surface-chemisorbed oxygen by formation of the valance Fe^{2+} and Ti^{3+} ions. The adsorption of methylene blue and the photoabsorption threshold of the nanotubes were greatly enhanced by the reductive annealing. 1 mol% Fe doping and reductive annealing produced the highest adsorption and photocatalytic efficiency for degradation of MB solution; extreme Fe doping decreases the photocatalytic efficiency. Moreover, the action mechanism of the Fe doping and reductive annealing was discussed.

Wednesday, 21/Aug/2019 5:51pm - 6:03pm

Abstract ID: 236 / FC: 10

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalysis and Energy

Keywords: Copper, Copper oxides, CO2 reduction, Water splitting, Solar energy.

Copper and Copper Oxides Based Materials for Solar Energy Conversion

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Energy conversion such as CO₂ reduction to fuel and water splitting with solar energy needs catalysts with high activity and good stability. Nanostructured materials are promising for future application in this research area. Although there are a large number of related publications, the issue about the catalysts has not been well addressed. So far, copper and copper oxide materials have been widely used as the catalysts for electrochemical, photochemical and photoelectrochemical CO₂ reduction. Additionally, metal copper as a good conductive material works well for electrode substrate. In order to take advantage of copper and copper oxide materials, we have prepared nanostructured copper and copper oxides based materials for photochemical, electrochemical and photoelectrochemical CO₂ reduction to organic fuel. Besides, copper nanowires have been used as the substrate to fabricate a highly efficient three-dimensional (3D) bulk catalysts of core-shell structure (Fig. 1), in which NiFe and CoFe layered double hydroxide (LDH) nanosheets were grown on the substrate cores supported on Cu foams, toward overall water splitting. The preliminary conclusion can be reached that after modification and deposition, copper oxides are prospective for photochemical and photoelectrochemical CO₂ reduction under solar light and the 3D core-shell electrocatalysts significantly advance the study for large-scale practical water electrolysis.

Abstract ID: 237

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Theory of Structure, Surface and Interface of thin films

Keywords: scattering, PBRDF, Mueller matrix, micro roughness films system, nanoparticles

Research on full-polarization light scattering characteristics from periodic nanoparticles upon micro roughness films system

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With the rapid development of microroughness film, various functional materials and devices emerge in endlessly. The detection and control of the optical dielectric film roughness is the most important research focus and hotspots about the preparation, test as well as performance evaluation of the optical film and the nanometer structural material. Focusing on the full-polarization light scattering characteristics of surface and the Mueller matrix bidirectional reflectance distribution function (BRDF), we will make some breakthroughs in theories and key technologies as following. We describe the surface scattering mode description and extend it to all elements of the Mueller matrix. The results are discussed by describing some metrics for the scattering behavior that are evaluated. The data show good agreement with theoretical predictions for different nanoparticle diameters and thin film thicknesses when bidirectional ellipsometry was employed to measure nanoparticles on Si wafers with different film thicknesses. The particle configuration extends from a single to a period. The scattering contribution of periodic nanoparticles or the micro roughness films is presented. Additionally, the information gained from these results should prove useful for the development of the nondestructive examination and optical performance design of nanometer structures.

Wednesday, 21/Aug/2019 5:24pm - 5:36pm

Abstract ID: 238 / FBB: 8

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biomimetic materials

Keywords: Magnetorheological fluid, superparamagnetism, microswimmer, flexibility

Effect of Flexibility on the Microswimmers Made of Functional Fluid

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Magnetorheological (MR) fluid is an artificial and functional fluid consisting of superparamagnetic microbeads suspended in a non-magnetic solvent. These superparamagnetic particles are applicable to reversible microdevices in biotechnical applications, such as micromixers, microswimmers, and other microfluidics. To effectively manipulate the locomotion of magnetic microbeads swimmer in the low-Reynolds number environment, the effect of flexibility on the propulsive efficiency of the swimmers composed of the superparamagnetic particles subjected to an oscillating field are investigated experimentally. The overall field is composed of a homogeneous static field H_d and a dynamical sinusoidal field H_y with a maximum amplitude H_p and an adjustable frequency f , that is, $H_y = H_p \sin(2\pi ft)$. The flexibility of the swimmer can be determined by the value of C_{max} , a dimensionless ratio of the diameter of the magnetic particle to the swimmer's radius of curvature. We designed two types of swimmers with higher propulsive efficiency and compared their flexibility with each other. L2S2 represents the swimmer comprising two large and two small particles and L1S3 indicates the swimmer composed one large and three small particles. Both swimmers were initially manipulated at a low frequency of $f=1$ Hz, then the frequency was gradually increased to 10 Hz for the acceleration of the swimmer. At the frequency of $f=10$ Hz, both swimmers accelerated to the maximum velocity and moved with constant speed afterward. The result shows that the maximum velocities of L2S2 and L1S3 are approximately $2.25 \mu\text{m/s}$ and $1.26 \mu\text{m/s}$, respectively. Additionally, C_{max} for each swimmer raises when the frequency is increased and gets to the maximum value of $C_{max} = 0.4$ and 0.3 at $f=10\text{Hz}$ and 7Hz for L2S2 and L1S3, respectively. This study proposes that microswimmer with specific configuration has the highest flexibility in certain field conditions, which may result in the best propulsive efficiency of the swimmer. The further discussions on the effects of the other controlling parameters on the flexibility of the swimmer are shown in full paper.

Abstract ID: 239

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Lithium Ion Batteries

Keywords: Lithium - ion, Sodium-ion, Carbon paper, Layered, Olivine

Newer Materials for Futuristic Energy Storage Devices

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The lithium ion battery has evolved as the major power source ever since its discovery in 1991 by Sony and represents one of the major successes of materials electrochemistry. Lithium ion batteries are becoming more and more popular in view of the multifarious applications arising from their high voltage and high power leading to light weight and smaller size cells/batteries. In view of the growing day to day demand for lithium ion batteries, intensive research is being pursued globally to develop new high performing cost effective electrode and electrolyte materials and importantly without compromising on environmental issues. Further, sodium ion batteries are emerging as an alternative to lithium ion cells owing to its low cost and abundance.

In my talk, I shall give you an overview of the recent developments in the area of cathode and anode materials. Details regarding the synthesis and characterization of high voltage (up to 5V) cathode materials based on layered and olivine materials shall be presented. Normally, graphite powders are employed as anode materials but we demonstrate a new type of lithium ion battery carbon paper replacing the conventional graphite powder coated on to a copper foil exhibiting high performance even at high rates (2C) when cycled between 2.9 and 4.1V and finds applications in LED lighting etc. These cells could be charged by solar energy. Moreover, our recent work on the development of electrode materials for sodium ion batteries shall also be highlighted.

Abstract ID: 240

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalysis for Chemical Synthesis

Keywords: Selective oxidation, toluene, nano-gold, catalyst

Selective oxidation of toluene with O₂ catalyzed by supported nano- gold catalysts

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Selective oxidation of toluene with O₂ catalyzed by supported nano-gold catalysts

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Selective oxidation of toluene to benzaldehyde has been eye-catching in academia and industry due to the increasing demand for chlorine-free benzaldehyde [1]. However, the yield of benzaldehyde were often low, and the atomic economy was poor because of the inertia of toluene to oxidation. Thus, in recent years, much effort had been paid to explore catalytic oxidation process for toluene, and the key issue was the design of effective catalysts.

Up to now, many promising catalysts had been synthesized for this conversion, especially using green oxidants of "O₂" or "H₂O₂" in absence of organic solvents and additives. However, the yield of benzaldehyde was still less than 10% [2]. Thus, there was still an urgent need to develop effective catalysts for the selective oxidation of toluene to benzyldehyde.

Here, a series of mesoporous oxides were synthesized by template column ion method, and then were used to support the nano-gold particles. X-ray diffraction and N₂ adsorption/desorption confirmed that the prepared supported nano-gold catalysts still exhibited typical mesophases. TG/DTA demonstrated that the catalysts held a high thermal stability even at a high temperatures of 1073K. The SEM images showed that nano-gold particles had been successfully loaded onto the mesoporous mixed oxides. Moreover, the obtained supported nano-gold catalysts exhibited high catalytic performance in the selective oxidation of toluene to benzaldehyde. Under the optimal reaction conditions, the highest toluene conversion reached 22.6% with 100% of the selectivity to benzaldehyde. Moreover, the catalytic performance remained after being recycled 10 times.

Fig. 1 N₂ sorption isotherms and pore-size distributions of Au/I/CuMgAlO Fig. 3 Catalytic performance of Au/I/CuMgAlO in the selective oxidation of toluene

Keywords: Selective oxidation, toluene, nano-gold, catalyst

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Abstract ID: 241 / Poster: 34

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Nanogenerators and self-powered nanosystems

Keywords: amorphous carbon coating, nanogenerator, durability, energy harvesting

Study on amorphous carbon coatings as a dielectric material for triboelectric nanogenerator

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Harvesting environmentally available energy is an emerging field. Scientists have been exploring new possibilities to reduce the dependencies on the fossil fuels and chemical batteries. Energy scavenging from the external environment such as wind, solar, thermal and kinetic energies have encouraged new technologies to power micro/nanosystems. The area of nano energy has exploded ever since, producing reliable and sustainable technology for harvesting power. Triboelectric nanogenerator (TENG) with its efficient, cost-effective, and ease of fabrication has seen a major participation in producing the nanopower. Ever since TENG was first reported in 2012 [1,2], many such devices have been developed to harvest natural energy using sliding and rotational motion. However, the efficiency of TENG lies in the dielectric materials used and its ability to reproduce the power at a consistent rate with minimum frictional losses between the moving surfaces. Thus, it is imperative to have a low friction material as dielectrics for the realization of durable sliding TENG. In the current study, we have illustrated the capability of amorphous carbon films as a potential dielectric material for TENG applications. Carbon is considered a unique and fascinating material of the 21st century due to its availability in different allotropes (graphite, diamond, and amorphous forms) and its physical properties which depends on their microstructure. amorphous carbon film possess some distinctive mechanical and physical properties such as chemical inertness, high hardness, corrosion resistance, low friction coefficient and high electrical resistivity. In this paper, amorphous carbon film-based TENG was developed to convert vibrational energy into electrical energy using amorphous carbon film as one of the dielectric materials. We have proposed that amorphous carbon film, with its outstanding tribological and mechanical properties, could play a major role in enhancing the durability of the TENG. Amorphous carbon films were deposited on the substrate using plasma-based ion implantation and deposition (PBII&D) technique and evaluated against conventional dielectric materials for improved efficiency. This paper proposes the potency of amorphous carbon films to be an efficient triboelectric material for realization of durable sliding TENG applications for the future.

Abstract ID: 242

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Applications of low dimensional, nano and 2D materials

Keywords: Nanofluids, transformer oil, thermal properties, heat transfer

Effects of ceramic nanoparticles on thermal properties of mineral transformer oil in nanofluids based on Al₂O₃ / AlN

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Transformer oil aging accelerates due to such parameters and factors: type of oil, system impermeability, water content in oil, working temperature and dirt type and quantity. Thermal properties are key in processing of the transformers and further maintenance. Heat transfer property of the transformer oil can be enhanced with the utilization of Al₂O₃ /AlN ceramic nanoparticles. Researchers have found that adding nanoparticles in liquids changes thermal conductivity, heat transfer properties and viscosity. Studies carried out had used Al₂O₃ as the nanoparticles and ethylene glycol, water, pump oil as base liquid to reach liquid like behavior with particles in them. Where the term nanofluid emerge to represent the unique changes in heat transfer properties of base liquid in comparison to liquid mixed with nanoparticles. As the solid nanoparticles have higher thermal conductivity than liquid transformer oil, the nanofluid on the basis of transformer oil and Al₂O₃ /AlN ceramic nanoparticles has altered thermal properties. Enhancing transformer oil heat transfer properties will maximize the autonomous work time of the transformers, by minimizing the time spent for the maintenance. The comparison of the transformer oil thermal properties and the nanofluids on the basis of ceramic Al₂O₃ /AlN nanoparticles shows clear difference. Further investigation is to compare the nanofluids itself by changing the percentage of the nanoparticles added in base liquid. Laboratorial activities with Al₂O₃ in different liquid substances-water, pump oil, ethylene glycol and engine oil by volume fraction gives correlation with thermal conductivity. Bigger the volume fraction higher the thermal conductivity. Increasing the thermal conductivity of the base liquid enhances heat carrying properties. For the case of transformer oil, Al₂O₃ having dielectric properties as well, insulates electricity from ambient, as well enhances heat transfer from heated parts.

Wednesday, 21/Aug/2019 4:24pm - 4:36pm

Abstract ID: 243 / FBB-2: 3

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biomimetic materials

Keywords: MXene, Noble metal nanoparticles, Biosensing, Extracellular Monitoring, Flexible devices

Flexible Biomimetic Sensors for Extracellular Monitoring Based on Freestanding MXene Film with In-situ Growing Noble Metal Nanoparticles

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Flexible biosensors currently have stimulated intense research in the construction of miniaturized and integrated detection system apply in implantable devices, compact diagnostic platforms, and portable lab-on-chip devices. We report here a new approach to build a flexible biomimetic sensor by rapidly in-situ growing high-density noble metal nanoparticles without reductant on a freestanding MXene film (Scheme 1). This strategy mainly benefit from the application of MXene, an emerging family of 2D transition metal carbides and nitrides, which is of attractive mechanical and electrochemical performance in the fabrication of flexible freestanding electrode substrates. Besides, the active functional groups of MXene possess strong reducibility for the construction of noble metal nanoparticles. This novel design of flexible electrodes provide new insight into biosensing, high sensitivity and favorable selectivity of the fabricated flexible electrode enables its use for extracellular monitoring of H₂O₂ secreted by live cells, and the excellent mechanical property resulted from the biomimetic structure of MXene film also ensures the further application in bioelectronics and point-of-care medical products.

Abstract ID: 244

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Applications of low dimensional, nano and 2D materials

Keywords: Nanofluids, Reynolds number, heat transfer, coolants

Technical problems of nanofluid research

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The article discusses the prospects for the use of nanodispersed liquids (nanofluids) as heat carriers. Briefly describes the properties of NA, options for use in various industries.

Summarizing, we can conclude that nanofluids are certainly promising coolants, with the help of which it will be possible to significantly reduce the metal consumption of aggregates, increase the safety of their use in emergency transient modes, accompanied by boiling. For the practical use of nanofluids as heat transfer, it is extremely important to have a clear idea of the mechanism of convection, especially forced.

In general, the results of experiments on the study of forced convection in nanofluids demonstrate an increase in the heat transfer coefficient relative to the base fluid under similar conditions, but the dependence is non-monotonic:

- at Reynolds numbers more than 9000 - optimum ;
- at concentrations of bass more than 3-4% vol. - also optimum .

An interesting fact is that an increase in the thermal conductivity of an NC relative to the base fluid is not the prevailing factor in the case of intensified heat transfer during forced convection.

Studies of heat transfer with free convection showed disappointing results - the heat transfer coefficient is usually lower than in the case of the base fluid. The reason for this is almost certainly the increase in viscosity of the medium.

The development of the science of nanofluids is still in the initial stage; therefore, it is necessary to conduct further comprehensive experimental studies of their properties, theoretical analysis, and compilation of general calculated correlations.

Abstract ID: 245

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Computational modeling and simulation of low dimensional, nano and 2D materials

Keywords: Cellulose, fibers, block formation

The production of cellulose fibers

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The production of cellulose fibers is carried out in suspension with water at a consistency of up to 60%. Consistency is the percentage by weight of the cellulosic material in the mixture of cellulosic material and water. One serious disadvantage of using cellulosic fibers is the difficulty of obtaining dry cellulosic fibers without reducing their dispersibility in an aqueous medium and / or their hardenability. This difficulty is similar to the difficulty of drying other cellulosic microfibrils or nanofibrils or even wood fibers in the traditional way and due to so-called keratinization. Hornification is caused by many factors, which include: the formation of irreversible hydrogen bonds (H-bonds) and / or the formation of lactone bridges. Keratinization leads to dried cellulosic fiber that cannot be re-dispersed in water, aqueous solution, or aqueous suspension, such as wood and paper suspension, when dry cellulose fibers are mixed with wood pulps in a shredder or in a checkerboard blend to be used as reinforcing paper additives. Each of these approaches has its drawbacks. In the case of the first approach, to reduce keratinization, MFC is dried with additives that block the formation of H-bonds and help prevent the formation of H-bonds and the lactone bridge. These supplements include sucrose, glycerol, ethylene glycol, dextrin or carboxymethyl cellulose. Here the main disadvantage is the large number of required additives, in some cases more than 15% wt. Are used. The second approach to reducing keratinization in the MFC and NFC during the drying process involves the derivatization of microfibrillated or nanofibrillated cellulose by introducing various groups, including carboxyl groups. However, derivatization requires the use of large amounts of reagent, for example, 5.81 g of monochloroacetic acid (MHC) (7.26 g of 80% MHC) per 36 g of MFC in isopropanol and aqueous solution under nitrogen atmosphere. It has not been established that MFC, derived from MHC or other molecules, can be re-dispersed in water after drying.

Abstract ID: 246

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk**

Topics: Alloy anodes

Keywords: Photovoltaic effect, Photoelectrochemical solar cells, Ternary alloy, XRD VU-Vis absorption.

Cd_{1-x}Zn_xSe/PVA Nanocomposite Functional Material for Energy Conversion Device

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The solar cells represent promising renewable solar-to-electrical energy conversion devices. The need for cheap, high-performance solar cells is of great importance for the world to be able to meet its growing energy demands. The present investigation is related to photovoltaic study of the Cd_{1-x}Zn_xSe nanocrystals embedded in polyvinyl alcohol matrix in photoelectrochemical cells.

The Cd_{1-x}Zn_xSe/PVA nanocomposite films for different composition of x, have been prepared by environment friendly single step solution method using polyvinyl alcohol as matrix. The color of Cd_{1-x}Zn_xSe/PVA nanocomposite films is found to change by varying the content of Zn and Cd. The structural and morphological studies have been done by the X-ray diffraction and Scanning electron microscopy. XRD result reveals that on increasing value of x in the composite, Cd atoms are replaced by Zn atom. Initially at x=0.0 hexagonal structure is obtained; on increasing value of x above 0.5 phase transition take place and cubic crystals are formed. Crystallite size estimated from Debye-Scherrer formula indicates that for higher x value, smaller particles are obtained. Crystallite size was obtained in 3.5 to 5.4 nm range from XRD result. SEM study reveals that the Cd_{1-x}Zn_xSe nanoparticles are well dispersed in polymer matrix with large agglomeration.

Optical absorption spectra of the films show that on increasing x in ternary compound, absorption edge shifts to lower wavelength resulting increase in band gap from 1.98 to 3.50 eV. Particle size of ternary alloy Cd_{1-x}Zn_xSe in PVA matrix has been estimated by absorption spectra using effective mass approximation and found to be nearly same as that from XRD. Photoelectrochemical cells were fabricated for photovoltaic studies in which Cd_{1-x}Zn_xSe/PVA nanocomposite films were used as photo-electrodes. The photovoltaic study was carried for different composition of x in Cd_{1-x}Zn_xSe/PVA and effect of annealing process on photovoltaic performance of nanocomposites has been investigated. The photovoltaic studies show that with changing the zinc content in Cd_{1-x}Zn_xSe/PVA, maximum efficiency is obtained for x=0.75. The structural, morphological, optical and photovoltaic properties of the Cd_{1-x}Zn_xSe/PVA nanocomposites are influenced by annealing time and annealing temperature also. The best performance in terms of smaller particle size, band gap, surface structure and highest photovoltaic efficiency has been obtained at 150°C and 1½ hour annealing.

From our study it can be said that ternary alloy Cd_{1-x}Zn_xSe/PVA nanocomposites are good candidate for photoelectrochemical cell due to their interesting properties of band gap modulation as well as size quantization. Polymer matrices provide easy and controlled processability, in terms of growth and morphology, which is very suitable for photovoltaic cells.

Abstract ID: 247

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Additive manufacturing Applications

Keywords: Shape deformation, Actuation, 3D/4D Printing, Additive Manufacturing

3D printing of shape-morphing architectures from bilayer to homogeneous material

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Facile preparation of architectures with precise control of shape deformations are crucial challenges due to the complicated process technique and harsh demands of the active materials. To address, the emerging three-dimensional (3D) printing is employed to build programmable shape-morphing architectures. Two kinds of shape-morphing architectures with bilayer structure and homogeneous materials were developed with FDM and DLP 3D printing technology, respectively. In the former, bilayer paper-based photothermal shape changing actuators were realized with FDM 3D printing of polylactic acid (PLA) and multi-walled carbon nanotubes (MWCNTs) composite. It was found that the paper-based bilayer actuators that possess photo-triggered shape changing properties with deformation under near infrared irradiation and recovery once the light source switched off. In the latter, architecture hydrogels with complex and controllable shape deformation that is composed of only hydrogel were built with Digital Light Processing (DLP) 3D printing. The basic principle is that the secondary microstructures introduced in the side of hydrogel strips can induce the bending or twisting deformations due to the asymmetrical swelling. With the merits of freeform design and fabrication, various hydrogel architectures including strips, sheets and 3D objects are built with stereolithography-based 3D printing, which realize complex, controllable shape deformations via the programmed microstructures on feature surface, such as bending, twisting, and even mimicking plant cirrus or petals. It is believed that the facile 3D printing strategy for shape-morphing architectures will provide tremendous opportunities for the design and fabrication of soft robotics, actuators and other devices where programmable shape deformations are required.

Abstract ID: 248 / Poster: 35

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Polymeric composites

Keywords: Conductivity, Carbon Black, Polymer Blends

Highly efficient conductive networks formed by selective localization of carbon black at the interface of sea-island structured polymer blends

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Highly efficient conductive networks formed by selective localization of carbon black at the interface of sea-island structured polymer blends

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Polymer/carbon black (CB) composites have been widely used in industry as antistatic and conductive materials. In dealing with the high electrical percolation thresholds that bring high cost and probably adverse effects on other properties, the search for means to build up highly efficient conductive networks of CB in polymer matrices has long been an interesting research subject. It is well-known that highly efficient conductive networks can be formed by the selective localization of conductive fillers at the interface of continuous polymer blends. However, very limited work concerns the formation of conductive networks through the selective localization of conductive fillers at the interface of sea-island structured polymer blends. We observed that the electrical percolation threshold of carbon black (CB) in thermoplastic polyurethane (TPU) decreased by 46% with the addition of 20 wt% polyamide copolymer (COPA) and that in polyamide MXD6 decreased even to a much greater extent with the incorporation of 20 wt% PET through selective localization of CB particles at the interface of sea-island structured TPU/COPA and MXD6/PET blends, respectively. The main driving force for the interfacial localization of CB particles is the strong and counterbalanced interaction of CB with the two types of polymer molecules during melt compounding. The CB particles bonded with both types of molecules can act like Janus particle-type compatibilizers. Highly efficient conductive networks are formed through the CB-covered domains and short inter-domain distances. Furthermore, we found that this type of conductive network can be used to make POM/TPU blends conductive at low CB loadings by the addition of a minor PA6 component and formation of a hierarchical structure composed of minor PA6 as droplets inside one major TPU phase and CB localized at the PA6/TPU interface. This work demonstrates that the selective localization of conductive fillers at the interface of sea-island structured polymer blends is also a viable approach to build up highly efficient conductive networks.

Key Words: Conductivity, Carbon Black, Polymer Blends

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Abstract ID: 249

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Biocomposites

Keywords: cellulose, nano, composites, energy, biopolymer

Nanocellulose based Functional Composite Materials

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Bio-derived polymer composites have gained tremendous attention in recent years. Cellulose, a natural polysaccharide is one of the most widely used biopolymers owing to its physical and chemical properties, biodegradability etc. The ability to convert cellulosic materials from waste biomass to nanometer sized fibrils has led to new properties and applications. Nanocellulose refers to two different types of nanomaterials: short, low aspect ratio cellulose nanocrystals or cellulose nanowhiskers (CNC or CNW) and long, high aspect ratio cellulose nanofibrils (CNF). CNCs and CNFs are attractive as mechanical reinforcements and rheology modifiers. We will present here our efforts to tailor the morphology of CNC and CNFs and how their properties can be leveraged in controlled release nanocomposite systems, ferroelectric energy harvesters and mechanically tough biodegradable composites.

Thursday, 22/Aug/2019 12:03pm - 12:15pm

Abstract ID: 251 / FLNM-2: 6

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

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

Keywords: silver nanowire, metallic MoS₂ nanosheets, nanocomposite, stretchable strain sensor, triboelectric nanogenerator.

Highly Conductive Composite Film of Silver Nanowires Network “Nanosoldered” by Metallic MoS₂ Nanosheets for Stretchable Strain Sensor and Self-powered Triboelectric Nanogenerator

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The growing demand of real-time monitoring of human health has triggered the rapid development of flexible and wearable devices. Particularly, highly stretchable, stable, and wearable strain sensors that can be easily mounted on clothing or directly attached to the body for monitoring various physical parameters are urgently needed to obtain accurate signals. Herein, we fabricated a highly flexible and stretchable strain sensor with a sandwich structure, where a composite film is embedded between two layers of PDMS (Scheme 1). The highly conductive composite film was fabricated based on silver nanowires (AgNWs) network modified with metallic MoS₂ nanosheets. This mixed-dimensional structure (1D–2D) composite film with excellent properties combines the flexibility of 2D MoS₂ nanosheets with conductive and stretchable 1D AgNWs network. In addition, the large surface area, mechanical flexibility, and strong bonding with AgNWs enable the metallic MoS₂ nanosheets to wrap around and nanosolder the AgNWs junctions, which could significantly reduce the resistance of the composite. Results show that AgNWs-MoS₂ composite film-based stretchable sensor shows much higher stretchability and smaller resistance increase than that of only AgNWs under the same stress. This stretchable sensor can successfully be utilized to monitor a wide range of human motions in real time. More importantly, we find that this sandwich structured PDMS/AgNWs-MoS₂/PDMS device can be used as a triboelectric nanogenerator, which can convert mechanical energy into electricity and thus detect human motions without a power supply, providing a promising route to future wearable artificial intelligence with comprehensive tracking ability of real-time signals for human health applications.

Wednesday, 21/Aug/2019 5:36pm - 5:48pm

Abstract ID: 252 / FBB: 9

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Advances in Enzymatic and Non-Enzymatic Biosensors

Keywords: MXene, bimetallic nanoparticles, enzymatic biosensor, organophosphorus pesticides

A Portable Enzymatic Biosensor Based on Bimetallic Nanoparticles Modified Two-dimensional MXene Nanocarriers for Pesticide Detection

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As the new member of two-dimensional (2D) transition metal carbides and nitrides, MXene has exhibited promising properties in energy storage, electromagnetic interference shielding, catalysis, and sensor field. Based on its properties, we propose a portable and disposable enzyme-based biosensor for the detection of organophosphorus pesticide using 2D MXene modified screen-printed electrode (SPE). Using MXene as the reducing agent and substrate, the Au-Pd bimetallic nanoparticles can be successfully prepared via the in-situ reduction process, which can well enhance the catalytic performance and the immobilization of acetylcholinesterase (AChE). With the addition of organophosphorus pesticide, the activity of AChE can be inhibited, making the related electrochemical signals weaken. Therefore, pesticide residues can be detected by monitoring the inhibition degree of AChE. Compared with the traditional pesticide biosensors, this biosensor is of easy preparation, high sensitivity, and desired repeatability, which can offer a promising application for the rapid and real-time analysis of organophosphorus pesticides in agricultural products.

Thursday, 22/Aug/2019 2:00pm - 2:12pm

Abstract ID: 253 / FESC-2: 1

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Nanogenerators and self-powered nanosystems

Keywords: Triboelectric nanogenerator, PVA/MXenes nanofibers film, all-electrospun, silk fibroin

All-Electrospun Flexible Triboelectric Nanogenerator Based on Metallic MXenes Nanosheets

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With the increasing potential of wearable and flexible electronics, self-powered devices are desperately demanded to overcome the restriction imposed by traditional energy storage devices. Here, a kind of highly electronegative and conducting material of MXenes nanosheet has been innovatively integrated with poly(vinyl alcohol) (PVA) for electrospinning nanofibers membrane to fabricate flexible triboelectric nanogenerators (TEGs). The PVA which acted as skeleton making this MXenes-based nanofiber film possessing high mechanical strength and flexibility, which can be stretched, compressed, twisted, and deformed arbitrarily. Additionally, silk fibroin was chosen for electrospinning nanofibers membrane to serve as electron donor for TEGs as its great triboelectricity as well as biocompatible and biodegradable nature. Herein, in order to maximize the output voltage, we optimized the volume of addition for MXenes, the thickness of the PVA/MXenes nanofiber-based film, operation force, and operation frequency. Due to the large specific surface area of nanofibers, highly electronegative and conducting material of MXenes, and the outstanding capability of silk fibroin to donate electrons in triboelectrification, the all-electrospun nanogenerator shows extraordinary electrical performance, which possesses an highly peak power density, excellent stability, and durability. Beyond harvesting electrical power, the fabricated TEGs can also be utilized for real-time monitoring various types of body motion. Lastly, we use it powering electrowetting on dielectric (EWOD) chip to actuate droplet transport, which have great potential applications in the field of cell manipulation, clinical tests, DNA analysis, drug delivery, and so on. Considering their excellent triboelectric performance, ease of large-scale manufacturing, and environmental friendliness, this technology provides a promising solution for developing practical, flexible, and self-powered electronic devices.

Abstract ID: 254

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Environmental Catalysis

Keywords: Hydrogen storage, MOF, carbon materials, hydrogen spillover, Nickel nanoparticle, hydrogen economy

A Ni-carbon material derived from Ni-MOF74 for room temperature hydrogen storage

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This study shows that hydrogen storage can be accomplished at room temperature using a nickel nanoparticle-carbon hybrid material. The material was produced through the carbonization of Ni-MOF74 under an inert atmosphere. The Ni-MOF74 sample carbonized at 500 °C displays an improved hydrogen storage capacity of ~400 % compared to the parent Ni-MOF74 material, 0.088 vs 0.002 wt%, at 298 K and 1 atm. We believe that these Ni-carbon hybrid materials hold promise for hydrogen storage as they show potential for storage at room temperature, and it is believed to be cost effective compared to traditionally used hydrogen spillover catalysts.

Abstract ID: 255

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Advances in the Synthesis and Characterization of low dimensional, nano and 2D materials

Keywords: 2D materials, metal thiolates, semi-conductor quantum dots, mechano chemical processes, optical properties

2D metal thiolates as single source precursors for the preparation of semiconducting metal and bimetallic sulfide nanocrystals

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The search for two-dimensional layered materials has reached new peaks after the discovery of graphene. Recently, we demonstrated that metal thiolates, which exist as lamellar assemblies in the neat state, can be disassembled into individual molecular sheets simply by dilution in apolar organic solvents and these can form ultrathin metallic or metal sulfide layers on substrates upon heat treatment.¹ Interestingly, metal thiolates have all the ingredients, which are essentially required for the preparation of monolayer protected metal and metal sulfide nanocrystals (the inorganic metal or metal chalcogenide complex as core and organic molecule as shell) inbuilt in their structure. Therefore, we investigated them as possible precursors for the preparation of monolayer protected metal and metal sulfide nanocrystals (NCs). We followed two strategies for the same. In the first one the 2D metal thiolates were used as single source precursors for the synthesis of semiconducting metal sulphide nanocrystals via “solvo thermal–decomposition” in solution.² We also extended this approach to prepare a large variety of uniform-sized semiconducting nanocrystals of metal sulfides including PbS, CdS, ZnS, MnS, Ag₂S and CuS by grinding these metal thiolates with a novel sulphur source octyl ammonium octyl dithiocarbamate (C8DTCA) through a solvent less solid state mechano chemical grinding process.³ Apart from this, silver (Ag NCs) and ultra small gold nanocrystals (Au NCs) have also been prepared using the same solvent less green approach, by the simple and convenient solid state grinding of the corresponding metal thiolate with sodium borohydride. Extending this procedure further, we recently started exploring the possibility of first, preparing mixed metal thiolates (bimetallic metal thiolates) and (ii) using them as single source precursor for the synthesis of some important bimetallic sulphides like AgBiS₂, AgInS₂, and CuInS₂ etc.

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Thursday, 22/Aug/2019 8:30am - 8:42am

Abstract ID: 256 / FCM-2: 3

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Metal matrix composites

Keywords: Multifiber Composite, Copper, Functional Properties

Cu-Bi multifiber composite wire

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An increasing demand for wires characterized with the properties like electric conductivity and strength, maintained at high mechanical, electric and thermal loads, is observed in the industry. The copper wires can be divided into:

- wires with high mechanical properties and low conductivity,
- wires with low mechanical properties and high conductivity, and
- wires with thigh mechanical properties and high conductivity.

The last group is the most interesting - it's been a subject of the intensive research, however it is still a huge challenge for scientists and process engineers to combine such parameters. The wires made of Cu-Ag alloys can have a tensile strength above 1200MPa and electric conductivity over 40MS/m, therefore they meet such requirements well. However, they are expensive due to the high silver content as well as technologically difficult production process. Another good material are the Cu-Nb alloy wires. The production process is also challenging, since it requires the application of a high-temperature always can be applied in the most challenging processes. This paper is focused on the process of the production of the multifiber wires on a copper matrix with Bi fibers. The microstructure analysis, chemical composition in the micro-area as well as the problems associated with their production are presented in the paper.

Abstract ID: 257

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Applications of low dimensional, nano and 2D materials

Keywords: ZnO, Photocatalysis, Nano-architectures

Hierarchical ZnO Nano-architectures and their Photocatalytic Properties

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Semiconductor photocatalysis is a promising solution for many environment-related issues. Among various oxide semiconductor photocatalysts, ZnO has been intensively studied for degradation of organic pollutants due to its high quantum efficiency, nontoxic nature and low cost. Unfortunately, intrinsic ZnO can only absorb ultraviolet light (5–7% of the total sunlight) due to its wide band gap (3.2 eV), which limits the photocatalytic efficiencies for practical applications. Research is now mainly focused on developing ZnO photocatalysts with high visible-light driven photo-activities via band-gap engineering.

In this work, we present a facile ultra-rapid solution synthesis of ZnO nanosheets with high BET surface area along with rich oxygen-vacancy defects. The BET surface area of ZnO was simply tuned by salt-addition, through an electrostatic-controlled self-assembly mechanism. The results obtained by Raman, PL, XPS and ESR analyses indicated that the as-prepared nanosheets had much higher concentration of oxygen vacancies compared to ZnO nanoparticles. The increased BET surface areas achieved here contributed to the increase of surface oxygen vacancies, which could improve the visible-light absorption and act as active sites for photocatalytic reactions, leading to the enhancement of photocurrent and photocatalytic activities of the ZnO nanosheets under visible-light illumination. Hybridization of ZnO nanosheets with Ag₃PO₄ nanoparticles further improved the visible-light photocatalytic activity, which was attributed to the efficient charge transfer between ZnO and Ag₃PO₄ through energy level matching, suggesting a synergistic effect of surface oxygen vacancies and Ag₃PO₄ coupling.

Abstract ID: 258

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

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

Keywords: ZnO, nanocomposite, light activation, gas sensing

Light Activated Gas Sensing based on ZnO Nanocomposites

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Metal oxide semiconductors have been extensively utilized in gas sensing, among which ZnO was most studied due to its nontoxicity, low cost and chemical stability. In this work, we demonstrate light activated NO₂ and CH₄ sensors based on ZnO nanocomposites.

ZnO/PbS hybrid nanostructures were fabricated by loading PbS nanoparticles on ZnO nanorods. Compared with the ZnO nanorod based sensor, the ZnO/PbS based sensor exhibited higher response to NO₂ under infrared excitation at room temperature. The enhanced NO₂ sensing performance of the ZnO/PbS nanocomposites was attributed to the electron transfer from the narrow-bandgap PbS to the wide-bandgap ZnO under infrared excitation, which enhanced the radial modulation of the conduction channel of ZnO nanorods.

A visible light activated CH₄ sensor based on oxygen vacancy riched ZnO (OR ZnO)/Pd nanocomposites was also developed. The nanocomposites were synthesized by first preparation of OR ZnO through H₂ treatment(>250°C) followed by depositing Pd nanoparticles on the OR ZnO nanorods. The OR ZnO/Pd nanocomposites were sensitive to CH₄ at 80°C in the dark, while the pristine ZnO nanorods showed no response. In addition, the CH₄ sensing performances of the OR ZnO/Pd nanocomposite sensors could be greatly improved under visible light, which was attributed to the synergistic effect of the oxygen vacancies, Pd nanoparticles and visible light.

Wednesday, 21/Aug/2019 4:27pm - 4:39pm

Abstract ID: 259 / FC: 3

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalyst Design, Synthesis and characterization

Keywords: Conductive nanomaterials, Electrochemical conversion, Energy, Chemicals

Electrochemical Conversion of Energy and Chemicals Using Conductive Nanomaterials and Wettability

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The electrocatalytic conversion of renewable resources, such as electrical energy, CO₂ to chemicals and fuels, is a promising means to meet the most urgent technological goals of our time; namely, clean energy production and environmental remediation. Some of the current challenges for modern electrocatalysis are to improve microbial electrocatalysis, oxygen reduction reaction (ORR) and CO₂ electroreduction. Here, micro/nanostructured conductive materials have been developed for improvement of electrocatalytic activities by tuning wetting and electronic properties. PANI nanofiber arrays could act as a solid-state polymeric mediator for bacterial extracellular electron transfer (EET) by tuning PANI oxidation states. The surface wettability of the electrodes strongly influences the bacterial EET activity at a fixed external potential: the EET activity on a hydrophilic electrode is more than five times higher than that on a hydrophobic one. Hemin-doped PEDOT, PPy decorated graphene were fabricated for improvement electrocatalytic activity for ORR with better stability and free-from methanol crossover effect by tuning electron properties. The anchor Ag nanoparticles onto graphene-wrapped nitrogen-doped carbon foam acted directly as electrode for electrochemical reduction of CO₂ to ethanol, overcoming the usual limitation of low faradaic efficiencies and selectivity for C₂ products. The hydrophobic exfoliated MoS₂ (H-E-MoS₂) nanosheets are fabricated from bulk MoS₂ by a cost-effective ball-milling method, followed by decoration with fluorosilane. H-E-MoS₂ as cost-effective electrocatalyst is capable to directly reduce CO₂ and H₂O to tunable syngas production with a wide range of CO/H₂ ratio from 1:2 to 4:1.

Abstract ID: 260

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Advances in the Synthesis and Characterization of low dimensional, nano and 2D materials

Keywords: Nanostructures, Porosity, Pulsed laser deposition, Seeding-angle

Deposition and optical properties of crystallographically oriented porous ZnO nanostructures

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We have synthesized two series of crystallographically oriented porous nanostructures wurtzite ZnO on quartz substrate using pulsed laser deposition (PLD) at glancing angle. Deposition was made in two steps for both the series: i) seeding layer of ZnO was first deposited by PLD at different angles (seeding-angles) and ii) nanostructured vertical growth was made at glancing angle PLD. For series-1, the oxygen partial pressure (PO₂) was varied during step-2, but the seeding-angle was normal in geometry during step-1. For series-2, the seeding-angle was changed during step-1 without varying PO₂ in step-2. The prepared nanostructures were studied for the parametric effects on growth, porosity and optical properties. For series-1, N₂ adsorption-desorption isotherms and the surface analysis reveals the porous nature of nanostructures grown with varied PO₂. At PO₂ of 7.5 Pa, the surface morphology and growth of ZnO nanostructure is very different (Fig. a) and it changes gradually with higher PO₂ (Fig. b) without losing its crystallographic orientation along c-axis. The cross-sectional scanning electron micrographs confirm the growth of nanostructures like walls. For series-2, the nanostructures grown at lower seeding-angle exhibit better crystallinity and optical properties compared with the nanostructures grown at relatively higher seeding-angles. Room temperature photoluminescence reveal a strong band-edge emission with suppressed visible emission in these nanostructures which makes the samples suitable for the application of ultraviolet light detection. The experimental results indicate that the seeding-angle and the oxygen partial pressure during PLD are crucial parameters, which can systematically tune the properties of ZnO nanostructures.

Abstract ID: 261

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Applications of Biopolymer for Drug Delivery

Keywords: Polymeric Micelles, Dual-Responsive, Chemo-Photothermal Therapy

Dual-responsive polymeric micelles for chemo-photothermal combination therapy

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Over the past years, the combination of chemotherapy and photothermal therapy has turned out to be a potential method for cancer treatment. In this study, we developed a new pH and reduction dual-responsive polymeric micelles (PMs) based on amphiphilic copolymer, in which chemotherapeutic drug (DOX) and clinical photosensitizer (ICG) were co-encapsulated for both NIR imaging and targeted chemo-photothermal combination therapy. The dual-responsive PMs were stable during blood circulation due to the presence of PEG layer and accumulated in the tumor through enhanced permeation and retention (EPR) effect. After efficiently internalized by tumor cells by way of folate receptor-mediated endocytosis, triggered DOX release would respond to the acidic endosomal compartments and reduction environment. Meanwhile, ICG could enhance the cellular uptake of the PMs and accelerate the drug release when exposed to 808 nm NIR light. Furthermore, the dual-responsive multifunctional PMs could perform as great theranostic nanoparticles to achieve tumor-targeted NIR imaging and enhanced antitumor efficacy via synergistic chemo-photothermal treatment. Therefore, the designed dual-responsive Co-PMs were promising theranostic nanocarriers for versatile antitumor drug delivery and imaging-guided cancer chemo-photothermal combination therapy.

Abstract ID: 262

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Anodes and cathodes Materials

Keywords: MCMB, Core Shell, Lithium-ion Batteries

Core-shell structure of Si@C coated MCMB as high-performance anode materials for lithium-ion batteries

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Mesocarbon microbeads (MCMB), as a kind of commercial graphite electrode material, has a reversible capacity of only 300-340 mAh g⁻¹ [1,2]. Obviously, it has the same limitation as other graphite anode materials for high energy density battery. So, surface modification is an effective strategy to improve electrochemical properties of MCMB, such as preparation of MCMB composite materials, chemical oxidation, and acid intercalation [3,4]. In our work, core-shell structure of Si@C coated MCMB (MCMB@Si@C) was successfully prepared via the TEOs hydrolysis and a typical Mg reduction process. This peculiar structural feature of MCMB@Si@C not only improves the electrochemical performance of MCMB, but also reduces the volume swell of Si anodes during cycles. As anode materials, a typical sample of MCMB@Si@C exhibits a high reversible capacity of 650 mAh g⁻¹ at 100 mA g⁻¹ during the first cycle, good cycling stability and excellent rate capability. Furthermore, this approach is quite simple and less expensive, which may supply a practical way to prepare high-performance anode materials.

Abstract ID: 263

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Applications of Biopolymer for Drug Delivery

Keywords: Bubble-Generating, Indocyanine Green, Doxorubicin, Chemo-Photothermal Therapy

Bubble-generating polymersomes for synergistic chemo-photothermal tumor therapy

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Nano drug delivery systems provide an appealing combination strategy for co-encapsulating multiple drugs. Meanwhile, stimuli-responsive nanovesicles have great potential in tumor treatment. Designing a bubble-generating drug delivery system is very important for the synergistic chemo-photothermal tumor therapy. Here, we demonstrate the bubble-generating polymersomes, which can generate bubbles in response to low pH or hyperthermia, fabricating to simultaneously encapsulate chemotherapeutic doxorubicin (DOX) and photosensitizer indocyanine green (ICG) for the synergistic chemo-photothermal tumor therapy. In vitro drug release study confirmed that acidic environment and NIR laser irradiation could accelerate DOX release from the bubble-generating polymersomes (BG-DIPS). Cellular uptake study indicated that laser-induced hyperthermia highly enhanced endocytosis of BG-DIPS into 4T1-Luc cancer cells. In vitro cytotoxicity study demonstrated that BG-DIPS exhibited much higher cytotoxicity than free drugs under laser irradiation. In vivo biodistribution study indicated that BG-DIPS could accumulate in the tumor region, prolong drug retention, and increase photothermal conversion efficiency. Furthermore, in vivo antitumor study showed that BG-DIPS with laser irradiation efficiently inhibited 4T1-Luc tumor growth with reduced systemic toxicity. Hence, the formulated bubble-generating polymersomes system was a superior multifunctional nanocarrier for stimuli-response controlled drug delivery and combination chemo-photothermal tumor therapy.

Wednesday, 21/Aug/2019 4:36pm - 4:48pm

Abstract ID: 264 / FBB: 4

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: 3D Scaffolds

Keywords: carbon nanotubes, fibers, threads, nanomaterial assemblies

Tailoring Electrical Conductivity of Carbon Nanotube Threads During Assembly

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Dry spinning is unique method to assemble carbon nanotubes (CNT) into useful micro- and macro-format materials. Because it relies strictly in the CNT van-der-wall forces, it is an ideal technique for studying physical properties of CNT fiber assemblies in their pristine states. They are free of catalyst, uniform in length, with a comparatively narrow diameter distribution, and their assembly into thread does not require additional chemicals or solvents. Good quality drawable CNT arrays can be readily assembled into uniform diameter threads with great control over the number of CNTs incorporated into the thread assembly. This uniformity allows study the physical properties that result from changes that occur during fiber/thread formation. This talk will report trends of electrical resistivity and mechanical strength that resulted from alterations in their manufacturing parameters, allowing to change intrinsic physical properties of a material such as electrical resistivity. An order of magnitude electrical resistivity changes in the fiber has been observed due to simple difference in Turn/m applied during CNT fiber assembly. We correlate the electrical resistivity and mechanical strength as a function of diameter, density, and turns/meter. Understanding the effects of dry-spinning parameters will allow a better design of the physical properties of CNT threads for specific applications, such as strain or electrochemical sensors.

Wednesday, 21/Aug/2019 5:48pm - 6:00pm

Abstract ID: 265 / FCM: 10

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Industrial applications of composite materials

Keywords: propane-selective, adsorbent, adsorptive separation, propylene purification

Zirconium-Bipyridine MOF for the Selective Separation of Propane from Propylene

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The effective separation of propane and propylene mixtures at ambient condition is challenging in petrochemical industries. We report herein the propane-selective performance of Zr-based UiO-67-bpy (bpy = 2,2'-bipyridine) for the energy-effective separation of propylene and propane. The BET surface area of UiO-67-bpy reached 2280 m²·g⁻¹ with a pore volume of 0.69 cm³·g⁻¹. More importantly, UiO-67-bpy showed a preferential adsorption of propane over propylene with propane capacity of 9.70 mmol·g⁻¹ at 100 kPa and 273 K, resulted from the stronger interaction between propane and UiO-67-bpy through hydrogen bonds. The mechanism of the preferential propane adsorption on UiO-67-bpy was discussed with the help of DFT calculations, which revealed that the effective interaction through hydrogen bond between the hydrogen atom of propane and the nitrogen atom of bpy in UiO-67-bpy was formed, while the adsorption between bpy and propylene through hydrogen bond was weakened due to the repulsion of the lone pair on the nitrogen atoms in the bpy towards the electron-rich double bond of propylene, resulting in the preferential adsorption of propane over propylene with high propane capacity. Breakthrough experiment confirmed that the propane and propylene in binary mixture can be completely separated at room temperature using a fixed-bed with the UiO-67-bpy. Hence, this work demonstrates a feasible strategy to achieve the energy-effective separation of propane from propylene at ambient condition. Besides, the commercially-available bpy ligand contributes to the low cost of this strategy.

Abstract ID: 266

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Sol-gel and LB technology

Keywords: sol-gel process, abietic acid, epoxy resin

Development of Anticorrosive Hybrid Epoxy Resin Coatings

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Hybrid SiO₂-polymer matrix materials were prepared by silica particles and epoxy resin modified (MEF). An efficient and durable option against corrosion of metallic materials has been developed through the preparation and application of thin surface films made of finely disseminated SiO₂ colloidal particles, which are trapped inside either functionalized (MER) or unfunctionalized (ER) epoxy resin polymer networks. Impervious, resistant, and anticorrosive polymer coatings of purely resinous or resinous-inorganic natures are obtainable this way. Silica nanoparticles were synthesized by the sol-gel process and chemically inserted in a polymeric matrix having carboxylic end groups attached to its chains. The functionalization of the polymeric matrix has the purpose in situ of uniting these groups carboxyl groups OH of the surface of the silanol groups during the process sol-gel. The materials prepared were characterized by FTIR and Raman spectroscopy techniques. An assessment of the anticorrosive performance of each ER-SiO₂ and MER-SiO₂ coating, once deposited on the surface of Cu plates, have been made inside a misty saline chamber operated under accelerated corrosive conditions. The results of this test indicate that the anticorrosive efficiencies of the ER and MER-SiO₂ coating films are superior than those related to the ER and MER-SiO₂ coverings. Some relevant textural, morphological, and structural properties of the different types of coatings have been determined by FT-IR spectroscopy, scanning electron microscopy.

Abstract ID: 267

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Additive manufacturing Applications

Keywords: Metal patterning, room-temperature printing, hybrid material printing, high conductivity, flexible electronics

A Room-temperature High-conductivity Metal Printing Paradigm with Visible-light Projection Lithography

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Flexible electronics gain increasing significance in applications such as health monitoring sensors, new-generation flexible displays and circuits in recent decades. Fabricating flexible electronic devices requires integrating metallic conductors and polymeric insulators in complex structures precisely on heat sensitive substrates. Current metal-patterning methods such as evaporation and laser sintering require vacuum, multi-step processes, and high temperature during sintering or post-annealing to achieve desirable electrical conductivity, which damages low-temperature polymer substrates. Here reports a facile eco-friendly room-temperature metal printing paradigm using visible-light projection lithography. With a particle-free reactive silver ink, photo-induced redox reaction occurs to form metallic silver within designed illuminated regions through a digital mask on substrate with no significant temperature elevation (<4 C), allowing for the usage of many low-temperature substrates that otherwise cannot be used by conventional metal manufacturing methods and opening up the opportunities for many unprecedented functions of novel devices. The patterns exhibit remarkably high electrical conductivity achievable at room temperature (2.4×10^7 S/m, ~40% of bulk silver conductivity) after simple room-temperature chemical annealing for 1~2 s. The finest silver trace produced reaches 15 μm . Neither extra thermal energy input nor physical mask is required for the entire fabrication process. Metal patterns can be printed on various substrates, including PET, PDMS, polyimide, Scotch tape, print paper, Si wafer, glass coverslip, and polystyrene. By changing inks, this paradigm can be extended to print various metals and metal-polymer hybrid structures. This method greatly simplifies the metal-patterning process and expands printability and substrate materials, showing huge potential in fabricating (flexible) microelectronics with one system, avoiding expensive equipment, vacuum conditions, high manufacturing temperature and multiple-step processes in conventional metal patterning methods, and it also brings down the cost and time for metal printing.

Abstract ID: 268

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Optical, Optoelectronic and Dielectric Coatings

Keywords: biaxial molecular ferroelectric, high-K dielectric property, transparent flexible membrane, dipole moment of hydrogen bonds

In-situ Preparation of a Biaxial Molecular Ferroelectric / Polymer flexible films with High-K Dielectric Properties

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Dielectric capacitors with high dielectric constant and high energy storage density have drawn increasing attention¹⁻³. So far, plenty of efforts have been made to achieve high dielectric constant of polymer materials by adding high dielectric constant inorganic materials or conducting materials, such as ferroelectric materials, semiconductor, metal, and carbon nanomaterials. Some materials contain heavy metals and the preparation process usually require costly thermal vacuum processing, and large loading of fillers may aggregate and introduce more structural defects, and then reduce the transparency and flexibility of polymer composites materials, which will limit the application of those composite polymer materials. Here we report a high-K dielectric, flexible polymer film by in-situ preparation of biaxial ferroelectric molecule-incorporated polymer materials by spin coating of the mixture solution containing uniformly dispersed soluble dielectric crystals. With the addition of biaxial ferroelectric molecule, we can get functional thin film with different dielectric properties in different orientations. This study offers a promising route to greatly enhance the dielectric properties of ferroelectric molecule and provides suggestive insights for developing high-performance polymer thin films for electromechanical energy storage.

Abstract ID: 269

Symposium 6: Functional Thin Films (FTF)

Invited Talk

Topics: Ferroelectric film

Keywords: spintronics

GeTe(111) ferroelectric and (GeMn)Te multiferroic Rashba semiconductor: a novel paradigm for spintronic applications

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Manipulating spin textures through magnetic or electric fields is a timely issue due to the potential for applications in low power electronics. Ferromagnetic semiconductors have received continued attention because of the novelty of their fundamental properties and their use as a basis of future semiconductor spintronic technologies. In this respect a novel class of materials based on ferroelectric GeTe(111) enabled to combine ferroelectric order with Rashba type switching of spin textures at room temperatures [1]. With low Mn-dopings the system is expanding its functional properties by displaying Rashba-Zeeman type spin splitting below a $T_N \sim 110$ K. This novel class of materials, called multiferroic Rashba semiconductors, promise not only integration of ferromagnetic and semiconducting properties [2-4], but due to ferroelectricity from the host α -GeTe(111) they display Rashba-Zeeman type spin splitting coupled to ferroelectric order, with evidence of effective magnetoelectric coupling [5]. The system thus constitutes an intriguing route for a non-volatile and static electrical control of the spin degrees of freedom. Based on soft x-ray and VUV angle resolved photoemission studies in spin and momentum-resolved ways, combined with x-ray photoelectron-diffraction experiments, the limitations of the electric control of these Rashba type spin states is discussed. We found that besides ferroelastic and depolarization effects, a depth of six atomic layers below the GeTe surface significantly deviates from the expected truncated bulk structure, which we believe is affecting the electric control of Rashba type spin textures.

Key Words: multiferroic Rashba semiconductors, photoemission, photoelectron diffraction, spintronics

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Abstract ID: 270

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Hybrid cells for energy harvesting

Keywords: photo-ferroelectric, multi-source energy harvesting, piezoelectric, photovoltaic, KNBNNO

A multi-functional photo-ferroelectric ceramic for multi-source energy harvesting and sensing with only one component

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For nearly 40 years, photo-ferroelectric materials have been limited to theoretical studies due to either wide band gaps or weak ferroelectricity, leading to inefficient photovoltaic effects or insensitivity to light/electric/strain excitations, respectively. This issue then hindered the practical use of photo-ferroelectrics in multi-functional components. In this talk, a multi-functional ceramic material and multi-source energy harvesting component will be presented. It is based on a widely used lead-free ferro-/piezoelectric composition – $(K_{0.5}Na_{0.5})NbO_3$ (KNN), doped by Ni^{2+} and with oxygen vacancies present in the structure (abbreviated as KNBNNO hereinafter). The KNBNNO is able to exhibit a narrow band gap of 1.6 eV whilst maintaining the KNN-level ferroelectric, piezoelectric and pyroelectric properties. Such multi-functional properties enable the KNBNNO to be simultaneously used for visible-range (solar) photovoltaic and ferro-/piezo-/pyroelectric effects. It is the first materials of its kind discovered in history, and thus has combined the separate families of visible-range band gap semiconductors and strong ferro-/piezoelectric materials.

In order to demonstrate the utilization case and feasibility of the KNBNNO, an energy harvesting-sensing hybrid device has been fabricated and tested. It is able to simultaneously convert solar, thermal (temperature fluctuation) and kinetic energy into electricity. Furthermore, the harvesting and sensing functions can also be integrated in the same material/component, e.g. the DC photovoltaic signal for power source whilst the AC piezoelectric/pyroelectric signals for sensing, to achieve an energy efficient design.

Compared to conventional individual and hybrid energy harvesters/sensors, the benefit of using the KNBNNO is that multiple energy sources can interact with the device made from it without the need of increasing the complexity and size of the entire system. This will open doors for novel one-component, miniaturized multi-source energy harvesters as well as monolithic, self-powered and battery-less sensing systems. The interaction between the visible light and domain walls in the KNBNNO will also stimulate the development of next-generation opto-ferroelectric devices such as light-(re-)writable data storage distinguishing wavelengths.

Abstract ID: 271

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Additive Manufacturing & bioprinting

Keywords: Additive Manufacturing, Fatigue, Fracture, Notch, Surface Roughness

Fatigue assessment of additively manufactured light alloys for biomedical applications

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Additive manufacturing has recently attracted considerable attention and has promising applications in various industries. By manufacturing parts in a layer-by-layer manner, high geometric complexity can be achieved for a wide range of materials. One of the main challenges related to additively manufactured metals is to accurately predict the structural integrity of the respective components. The as-built components display rough surfaces containing defects, reported to reduce the mechanical properties. In the case of medical applications these surfaces has been proven to be beneficial in some applications. Here we evaluate the fatigue behavior of notched specimens of Ti6Al4V produced by selective laser melting. The results were compared to that of plain specimens. The interaction between geometrical discontinuities and material discontinuities has been extensively studied using experimental analyses. The studied specimens were chosen in a way to have similar geometries as the prosthesis used in biomedical applications.

Abstract ID: 273

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Nano-optics, Nano-optoelectronics, Nano-Photonics and Nano-photonics

Keywords: Nano, Nanophotonics, Plasmonics, Rare Earth, Imaging

Plasmon-Induced Optical Emission Enhancement of Trivalent Rare Earths in Hybrid Core-Shell Nanostructures

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Enhancing the optical properties and functionality of nanomaterials is of key interest for fields ranging from optoelectronics, to biomedicine and energy. We have developed multilayer core-shell fluoro-plasmonic nanoparticles composed of a plasmonically active metal layer used to enhance fluorescence of an outer rare earth based layer. A refined synthesis method enables tunability of the plasmonic enhancement through control of the layer dimensions. Substitutions in the rare earth layer provide a wide range of tunability of the fluorescence wavelength, as well as the addition of new functionalities such as magnetic properties or x-ray fluorescence through the inclusion of additional dopants. Electrodynamics simulations were used to design and experimentally tailor these hybrid structures, and experimental results from optical measurements were compared with the theoretical models. This research presents promising results for a new novel and highly tunable nanomaterial with enhanced optical emissions for applications including clean energy, theragnosis, imaging technology, memory, and data storage devices.

Thursday, 22/Aug/2019 9:42am - 9:54am

Abstract ID: 274 / FCM-2: 9

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Smart Composites

Keywords: Lignin, 3D-printing, self-healing, sensors, neutron scattering.

Multifunctional 3D-printing materials from modified lignins

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We report the transformation of a biorefinery waste stream, lignin, into value-added materials for additive manufacturing. The rigidity of hyper-branched phenolic lignin was modified with flexible semi-crystalline molecules revealing unique characteristics for 3D-printing, shape-programming and self-healing, as well as stress-strain sensing applications. The key to this material design is controlling inter- and intramolecular interactions and molecular relaxation of both amorphous and crystalline phases via the formation of multiple electron donor-acceptor complexes. Structural relaxation and evolution of the amorphous phase were investigated by in situ small angle neutron scattering. Removal and recrystallization of the crystalline phase were studied by in situ wide-angle x-ray diffraction. The details will be discussed in the talk.

Abstract ID: 275

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

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

Keywords: Self-assembly, Plasmon, Block copolymers

Block copolymer based self-assembled hyperbolic metamaterial in the visible range

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ASHOD ARADIAN¹, MORTEN KILDEMO³, VIRGINIE PONSINET¹**

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Nanophotonics explores the possibility of modulating light propagation with very small amount of matter using nanoscale phenomena. The occurrence of plasmons at metal/dielectrics interfaces is one of the very relevant phenomena, which has encouraged, in the recent years, active research efforts towards the fabrication of nanostructured metal-dielectric materials and surfaces. This presentation will show how we used self-assembling block copolymers for the “bottom-up” formulation of original anisotropic plasmonic nanocomposites. In particular, we produce and study periodic cylindrical and lamellar assemblies composed of nanometric domains of pure polymer and domains of composite of polymer loaded with a high density of gold nanoparticles. The spectral variation of their anisotropic effective dielectric permittivity is determined by spectroscopic ellipsometry using appropriate effective medium models. For large gold loading, the lamellar stacks present a frequency domain, in which the ordinary and extraordinary components of the dielectric function are of opposite signs. This peculiar property, called “hyperbolic”, allows for the propagation of large magnitude wavevectors, carrying details finer than half the wavelength, otherwise corresponding to evanescent non-propagative waves in a usual dielectric.

Abstract ID: 277

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin Films in Biological and environmental Applications

Keywords: Hydrogel, Thin Film, Optical Sensor

Hydrogel Thin Film Interferometer Sensor for Metal Detection

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With an increasing demand of real-time health and environment monitoring and prevalent smart technologies nowadays, high precision molecule detection with micro-sized devices is playing a vital role with many exciting progresses recently. For example, Ca^{2+} plays a critical role in the modulation of fundamental cellular processes; including cell proliferation, differentiation, and survival/death. Cu^{2+} is an essential trace element vital to the health of human beings. High intake of Cu^{2+} triggers aberrant oxidative damage and toxicity and causes serious health effects including diarrhea, stomach, liver damage, kidney disease and neurological diseases. However, the ICP-MS and AAS/AES methods rely on large instruments, complicated analyte pre-treatment, and trained operator, making them not suitable for real-time environmental monitoring. On the other hand, to synthesis conventional chemical sensors with high sensitivity and selectivity is time-consuming and expensive. Here we demonstrate a new colorimetric sensor platform based on a stimuli-responsive hydrogel thin film interferometer.^{1,2} The stimuli-responsive hydrogel thin films coated on reflective substrates show changes in their visually-detectable colors and shifts in their corresponding reflectance spectral peaks, as the consequence of film thickness changes in response to the different concentration of the analyte. This unique chemo-mechano-optical signal transduction mechanism has significantly amplified the nm-scale hydrogel thickness change to a greater and more sensitive optical spectrum change. The nature of the soft gel makes this platform transparent, flexible, stretchable, and compatible with a variety of substrates. This omni-directional sensing broadens the flexibility in applying the hydrogel interferometer platform on various usage scenarios. These showcase the promising potential in on-site analysis and even real-time monitoring of seawater or wastewater and in new point-of-care or health monitoring technologies, without the needs of complex procedures and costly large equipment required by current methods.

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Abstract ID: 278

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: encryption, anti-counterfeit, hydrogel

Reconfigurable surface for encryption and anti-counterfeiting

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Security technologies like anti-counterfeiting and encryption have found wide applications in identity cards, currency, tags and important documents. Traditional holographic anti-counterfeiting marks rely on the diffraction and/or interference of light on printed surfaces, therefore are static and easy to counterfeit. To meet the increasing demand for novel and enhanced anti-counterfeit/encryption materials, various functional materials that display distinct chemical, physical as well as optical and electrical properties have been investigated for dynamic anti-counterfeiting and info encryption purposes. However, dynamic and reversible solution for these security technologies with fast response and high contrast is still a challenge. Inspired by various creatures in nature that exhibit vivid and switchable color through adaptive periodic nano/micro-structured surfaces, here we demonstrate a reconfigurable surface that harnesses the high contrast aspect of structural colors combined with the fast and reversible response of hydrogels. Thus, dynamic, high contrast and fast encryption and anti-counterfeiting have been achieved.

Wednesday, 21/Aug/2019 4:24pm - 4:36pm

Abstract ID: 279 / FBB: 3

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Advances in Bioelectronics and Commercial biosensors

Keywords: Dielectrophoresis, Filtration effect, Matrix effect, Bio-fluid based diagnosis, Commercialized biosensor

High accurate bio-fluid based electrical biosensor for commercialization

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High accurate, sensitive and selective diagnosis of disease molecules in biofluid is an essential virtue for commercialization of biosensors. Most of biofluid is consisted of various matrix factors, which are easily absorbed that decreases an accuracy of biosensor. This unavoidable phenomenon is defined as a matrix effect in biofluid. Therefore, various methods have been suggested to decrease the matrix effect—general methods are as follows: using a surfactants such as Tween 20, or using a blocking agent such as BSA, or using a receptor with high affinity. A physical filtration through micro-fluidic channel is also one of the methods to alleviate the absorbed matrix factors. However, specifically engineered receptors with high affinity is difficult to access easily, and the blocking agent and surfactants have the possibility of increasing the complexity of an experiment which cause changes in the biosensor due to the blocking agents and surfactants themselves. In addition, physical filtration involves the risk that the target molecules may be removed with matrix factors. Therefore, a method that can be universally used and reduces the absorbed matrix factors without using physical removal, while maintaining the simplicity of the experimental procedure, is required.

Here, a novel high-accuracy biosensor through a filtration effect based on a dielectrophoresis (DEP) is suggested. The effect allows the biomolecules in biofluid to filtrate depending on a size: a target disease molecule—amyloid beta ($A\beta$)— binds to its antibody in a reaction region, while the matrix factors of larger than $A\beta$ are expelled from the region. Thereby, the matrix effect is decreased followed by improve the accuracy, sensitivity as well as selectivity of the sensor. Filtration effect was verified by measuring the impedance change of an interdigitated microelectrode (IME) sensor caused by reaction of $A\beta$ in (1) phosphate-buffered saline (PBS) and (2) standard plasma. Also, the impedance change was defined and calculated as a matrix effect factor (MEF) to express the influence of filtration effect more clearly. MEF was decreased approximately 78.12% by filtration effect, and this decrease discriminated between two types plasma from patients with AD and the normal control (NC) ($n = 10$ each): the impedance changes in the AD plasma were mostly increased by filtration effect, whereas the changes in the NC plasma were very minute. This difference was indicated as a disease evaluation index, and the average value of the indexes were approximately 1.52 ± 0.03 and 0.90 ± 0.03 in AD and NC plasma, respectively.

Our results demonstrates that filtration effect by DEP force attenuates the matrix effect in plasma, which subsequently enable to clear detection of disease molecules in real patient plasma. Consequently, the results implies that filtration effect may become a vital trigger toward commercialization of biofluid-based biosensors with high accuracy, sensitivity and selectivity.

Abstract ID: 280

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Ceramic based composites

Keywords: LD-pumped phosphor, Laser display, ceramic

Novel glass-in-LuAG ceramic with excellent luminous efficiency and high thermal stability for laser-diode-pumped phosphor

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Laser-diode-pumped (LD-pumped) phosphor has played a crucial role in application of laser display. The current commercial packaging materials of phosphors with weak thermal conductivity (0.1-0.4 W/m·K) and poor heat resistance (lower than 150°C), which are not suitable as high power density LD-pumped phosphor. To solve these problems, a lot of novel phosphors have been studied, such as glass, glass ceramic, phosphor-in-glass, transparent ceramic, etc. However, the so far reported phosphors cannot show strong pumped light absorption, high thermal conductivity, and heat resistance, simultaneously. This study presents a novel glass-in-LuAG (GIP) ceramic with excellent luminous efficiency (205 lm/W), high thermal conductivity (2.8 W/m·K at 80°C) and remarkable improvement in heat resistance (above 700°C) and reliability (luminous flux has only 0.5% drop after 100 h at 300°C). Furthermore, a Pb-free glass (25 wt.%) with good thermal conductivity (1.2 W/m·K at 80°C), high glass transition temperature (711°C) and high refractive index (1.84) has been designed as a high-temperature packaging material to fill the gaps of the phosphor powders, which can greatly enhance the thermal properties of GIP ceramic and reduce adverse light scattering. Those investigations show that the GIP ceramic is promising candidate for LD-pumped phosphor.

Thursday, 22/Aug/2019 9:36am - 9:48am

Abstract ID: 281 / FESC: 9

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrode/electrolyte interface phenomena

Keywords: Lithium ion battery, safety, cathode electrolyte interphase, Ni-rich

Quenching cathode electrolyte interphase on Ni-rich cathode materials for preventing short circuit problem in lithium ion battery

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In January 2017, Samsung announced the reason why the Note 7 explodes and losses of more than 5 billion US dollar. According to their explanations, it was caused by the internal short circuit problem in the lithium ion battery. Currently, there is no effectively solution for eliminating the internal short circuit problem owing to the sudden accident.

In this research, a new technology has been developed, which can be used to terminate the thermal runaway and promise the safety performance of lithium ion battery. High voltage Li-excess and Ni-rich layer-type cathode material is employed and combined with this safety electrode additive for investigation. In terms of the results, the new technology LIVING@ additive significantly enhances the cycle performance at 60oC and high voltage. In addition, the following figures illustrated that the battery containing LIVING@ technology is stable and passed the nail penetration test. On the other hand, the battery without LIVING@ cannot be used when the short problem is taking place. The LIVING@ contains self-polymerized hyper branch structure in order to insulate the directly contact between anode and cathode. This electrode additive not only provides high thermal stability on electrochemical reaction, but the columbic efficiency of charge-discharge is also enhanced.

Thursday, 22/Aug/2019 10:12am - 10:24am

Abstract ID: 282 / FESC: 12

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

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

Keywords: Continuum model, Gas storage, Gas separation, Nanoporous material, High-throughput materials discovery

Continuum model for gas storage in nanoporous materials

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There are increasing demands on novel materials for energy storage and flue gas separation. We describe a continuum model for calculating gas storage capacity directly from gas-sorbent interaction energies. In this continuum model, the chemical potentials of the external and internal gases are equal at adsorption equilibrium. Assuming near homogeneity of the adsorbed gas in the porous medium, thermodynamic properties such as the local pressure and density are obtained using the bulk gas equation of state. With increasing inhomogeneity of the adsorbed gas density originating from highly inhomogeneous gas-sorbent interaction, a density correction using a perturbative scheme is necessary. We show that our continuum model is accurate and efficient at both the room temperature and at low temperatures where the density inhomogeneity is large, and serves a promising tool for high-throughput materials discovery.

Abstract ID: 283

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Synthesis, Controllable Growth and Characterizations

Keywords: Nanowire devices, charge-transfer salts, electrodeposition, scalable manufacturing, mass transfer

Mass Transfer-Based Methods for Controlling the Growth of Charge-Transfer Salt Micro/Nanowires

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Nanowire sensors are promising to deliver greater performances than conventional sensors due to their size confinement. Despite their attributes, nanowire sensors have yet to play a significant role in the sensing market. This is in part due to the lack of scalable manufacturing methods, which require (1) scalable production of uniform nanowires and (2) the nanowires to be organized over large areas with controlled orientation and density. It has been recently discovered that charge-transfer complex wires, such as tetrathiafulvalene bromide ((TTF)Br) wires, show rapid and reversible conductivity changes in response to ammonia and other solvent vapors making them potential materials for gas sensing applications. Like other types of wires, it was a challenge to synthesize uniform (TTF)Br wires and organize them for sensor assembly. Here, we report a simple mass transfer-based method to address this challenge. We discovered that the use of Pt microdisk electrodes for electrodeposition of (TTF)Br wires resulted in wires with higher uniformity and aspect ratio than their counterparts deposited on Pt films. More interestingly, we found that the number of wires grown from a Pt microdisk electrode exhibited a limiting number of 3 or 4 per electrode when the electrode diameters are less than $\sim 1.4 \mu\text{m}$. Both experimental and simulation results suggest these are caused by the different TTF flux distributions at a microdisk versus a film electrode. The results have significant implications for scalable manufacturing of nanowire-based sensing devices.

Abstract ID: 284

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Composites in Innovative Applications

Keywords: Polyindole, Conductive Polymer, Gas Sensor, Composite

Graphene Based Materials/Polyindole Composites for Methanol Sensor

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Graphene based materials consisting of the commercial graphene, commercial graphene oxide, reduced graphene oxide, and synthesized graphene oxide were used to prepare composites with polyindole (PIn) as a methanol vapor sensor. The sensor testing was investigated by recording the electrical conductivity signal changes at room temperature. Herein, graphene oxide was prepared by the optimized improved Hummers method, called OIHM-GO, to compare with the commercial GO. The reduced graphene oxide was prepared by two different methods (thermally mild reduction and chemically reduction by ascorbic acid) using a commercial GO as a raw material. The composites were prepared by the in situ oxidative polymerization to obtain first the composite powder. Then it was compressed into a pellet form before methanol testing. The methanol response of the in situ GO/dPIn composite was higher than that of in situ OIHM-GO/dPIn, in situ C-rGO/dPIn, in situ T-rGO/dPIn, and in situ G/dPIn, respectively. The sensing mechanism depended upon the number of oxygen in the composite structure which induced the hydrogen bonding interaction with methanol molecules and increased the diffusion ability of methanol into the inner layer of the composites. The effect of OIHM-GO content of the composite on methanol response was investigated, OIHM-GO at 10 %v/v provided the highest conductivity relative response toward methanol vapor. The sensing material based on the in situ OIHM-GO/dPIn composite exhibited the sensitivity of 7.3712 ppm⁻¹ with the linear correlation coefficient (R²) of 0.9967 in the methanol concentration range from 1.14 - 11.36 ppm, and the theoretical LOD of 0.015 ppm. Moreover, the response was fully reversible and repeatable for at least 4 cycles with high selectivity. This work is the first report for preparing composite between polyindole and graphene based materials for sensor applications.

Abstract ID: 285

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Organic and polymer film

Keywords: schiff base, double-network, self-healing property, biological activities

Double network self-healing film and its Biological Activities

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Here, we report the fabrication of Schiff base-metal coordination-chelation interaction double-network films via Layer-by-Layer assembly technology. Novel double-network films based on Schiff base linkage resulted from the interaction between the aldehyde groups on the dialdehyde groups-modified poly (ethylene glycol) (DPEG) and the amino groups on chitosan (CH) as a primary network¹ and metal coordination-chelation interaction as a secondary network^{2, 3}, are fabricated based on layer-by-layer (LbL) self-assembly technology. Schiff base complexes of Cu²⁺, Zn²⁺ often show a good antibacterial activity against Gram-negative bacteria.^{4, 5} Calcium is the highest content of metal elements in the human body. Thus, Ca²⁺, Cu²⁺ and Zn²⁺ are selected to build metal coordination-chelation interaction in this paper. Dynamic Schiff base linkage and metal coordination-chelation interaction endow the films with the self-healing property to rebuild their structure and property. According to the results, the secondary network, metal coordination-chelation interaction, affected on the self-healing property. This data indicates that the order of the self-healing property from best to worst is as follows: (CH/DPEG) 15 film > (CH/DPEG) 15-Ca²⁺ film > (CH/DPEG) 15-Zn²⁺ film > (CH/DPEG) 15-Cu²⁺ film. Furthermore, the antibacterial and anticancer activity of double-network films is measured. According to results, the antibacterial and anticancer activities of double-network films are also affected by the metal chelation interaction. The activity data show that the double-network films exhibited different antibacterial and anticancer activities. The order is (CH/DPEG) 15-Cu²⁺ film > (CH/DPEG) 15-Zn²⁺ film > (CH/DPEG) 15 film > (CH/DPEG) 15-Ca²⁺ film. The Schiff base-bonded (CH/DPEG) 15 film and some Schiff base-metal coordination-chelation interaction double-network films have good antibacterial and anticancer activity. Thus, the self-healing double-network films are suitable for antibacterial and anticancer applications, and consequently, the study of self-healing, antibacterial and anticancer double-network films promises to greatly widen the biomedical applications of self-healing materials, such as in cancer treatment in clinical application as anticancer coatings.

Abstract ID: 286

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Design and application of composite structures

Keywords: metal-organic framework, TED@Cu-BTC, water stability, CO₂ capture, adsorption

Room-Temperature Synthesis of novel TED@HKUST-1 with enhanced water vapor stability for CO₂ capture

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As a new generation of porous materials, metal-organic frameworks (MOFs) are developing rapidly in recent years, and exhibit promising for applications in gas separation and storage, catalysis, sensing and detection because of their extremely high surface area, thermal stability, systematically tunable pore structure and chemical functionality. However, most MOFs are unstable under humid circumstances, which hinders their practical applications. Herein, we propose a new strategy to enhance the steam stability of HKUST-1. HKUST-1 was functionalized with 1,4-diazabicyclo[2.2.2]octane (TED) to yield TED@HKUST-1, which can be quickly finished within 1-minute at room temperature. The resultant TED@HKUST-1 showed BET surface area of 1421 m²/g, and high CO₂ adsorption capacity of 4.85 mmol/g at 1 bar and room temperature, which was well above that of ZIF-8, UiO-66 and MIL-101. More interestingly, after the materials were directly soaked in water for 54h, HKUST-1 completely lost its crystal structure, while TED@HKUST-1 still preserved its main crystal structure and 94.6% of its initial CO₂ adsorption capacity, suggesting that the water stability of TED@HKUST-1 was significantly improved. The origination of the improved steam stability of TED@HKUST-1 was interpreted by DFT calculations. In conclusion, the strategy of incorporating TED into HKUST-1 is very efficient in enhancing its structure stability due to the protection of Cu sites from TED.

Abstract ID: 287

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Composites in Innovative Applications

Keywords: Sulfonated poly(ether ketone ether sulfone) (S-PEKES) Sulfonated graphene oxide (S-GO); Polymer electrolyte membrane (PEM); Direct methanol fuel cell (DMFC)

Sulfonated (graphene oxide/Poly(ether ketone ether sulfone)(S-GO/S-PEKES) composite polymer exchange membrane for DMFC

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Sulfonated poly(ether ketone ether sulfone) (S-PEKES) was successfully prepared to obtain the currently highest degree of sulfonation of 0.744. Then, sulfonated graphene oxide (S-GO) was further incorporated into the S-PEKES matrix to increase the degree of sulfonation which significantly improved the membrane proton conductivity, permeability of methanol, and mechanical stability. The proton conductivity of the S-GO/S-PEKES composite membrane was enhanced 7 times higher than the commercial Nafion 117 membrane. Furthermore, S-GO exhibited additional positive effects namely the blocking of methanol crossover through the membrane, leading to a lower methanol permeability than Nafion 117 by two orders of magnitude, and the high mechanical stability.

Abstract ID: 288

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin films in Energy Harvesting and Storage

Keywords: 2D nanomaterials, Water purification, Energy harvesting

Functional boron nitride membranes and their applications in energy harvesting and water purification

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Two-dimensional (2D) boron nitride (BN) nanosheets, also called “non-carbon graphene”, consist of few layers of alternating boron and nitrogen atoms in a hexagonal arrangement. The polarity of BN bonds and the high surface area of h-BN-related nanostructures provide good adsorption properties of various substances ranging from organic pollutants to hydrogen. Nanostructured h-BN is therefore an ideal candidate as absorbent material.¹⁻⁴

In addition, significant efforts have been focused on the isolation and functionalization of BN nanosheets to achieve better dispersion, which would enable applications in optical devices, biological systems and composites. However, the concentration of the h-BN dispersions was typically below 2 mg mL⁻¹, even after long periods of intense ultrasonication. Therefore, the development of a practical high-yield process to achieve highly water-soluble BN nanomaterials remains a challenge. There is potential for h-BN, which is more oxidation- and intercalation-resistant than sp² carbon, to be used to produce similar structures. However, it is very difficult to achieve aqueous dispersion of h-BN using conventional routes. Here, we present a simple and efficient one-step method for the preparation and functionalization of few-layer BN by solid-state ball milling of commercially available h-BN and urea powders.⁵ The colloidal solutions of multi-layer h-BN can have unprecedentedly high concentrations, up to 30 mg/mL, and are stable for up to several months. They can be used to produce freestanding membranes simply by filtration. The functional BN nanosheets membranes exhibit good applications in super-thermal conductivity composites, nanofluidic device, molecular separation and Li-S batteries as a separator.⁶⁻⁹

Key Words: 2D nanomaterials, Water purification, Energy harvesting

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Abstract ID: 289

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Chemistry of 2D Materials for Energy, Catalysis and Sensing Applications

Keywords: bulk MOF materials, 2D MOF nanosheets, exfoliation, catalytic activity, hydrogen peroxide

Scalable production of two dimensional metal-organic framework nanosheets by shear exfoliation applied for colorimetric detection of hydrogen peroxide

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Two dimensional metal-organic framework (2D MOF) nanosheets, as a new member of the 2D family, have attracted extensive attention in recent years. MOFs are formed by coordination bonds between organic ligands and metal atom nodes with periodic structural units, which have advantages of well-defined chemical structure, convenient structural design and tunability. Compared with the traditional bulk MOF materials, 2D MOF nanosheets have higher surface area, more accessible active sites on the sheet surface, leading to higher activity in various catalytic reactions. The 2D MOF nanosheets can be prepared using ultrasonic exfoliation method and surfactant-assisted synthetic method. However, there are several shortcomings in previous reported methods, which limit its large scale applications. For example, the production yield of 2D MOF nanosheets using sonication method is low. The surfactant on the surface of 2D MOF nanosheets produced by the surfactant-assisted synthetic method will block the catalytic active sites, which decreases the efficiency of catalytic reaction. Therefore, for the first time, we exfoliated a serial of 2D MOF nanosheets (Zn-TCPP, Co-TCPP, Cd-TCPP, Cu-TCPP and Cu-TCPP(Fe)) using kitchen blender. The whole shear exfoliation process can be completed in 1 h and the yield of the 2D MOF nanosheets is quite high, which is suitable for the large-scale applications. Importantly, we demonstrated that the 2D Cu-TCPP(Fe) nanosheets have enhanced peroxidase-like activity compared with its bulk counterpart. Base on the excellent catalytic activity of 2D Cu-TCPP(Fe) nanosheets, a colorimetric method using 3,3',5,5'-tetramethylbenzidine (TMB) as substrate was developed for the detection of hydrogen peroxide with high sensitivity. These findings will have a profound impact on the preparation and sensing applications of 2D nanomaterials.

Abstract ID: 290

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Composites in Innovative Applications

Keywords: Poly(p-phenylene), Zeolite, Composite, Gas Sensor, Sulfur Dioxide

Poly(p-phenylene) and its Composites with ZSM-5, BETA, and 13X Zeolites as Selective Sensing Material for Sulfur Dioxide

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The interest in the development of composite materials as the new and alternative sensing materials has been continuing to replace metal oxide based sensors which operate at high temperature. Herein, we report the fabrication and operation of sensing materials based on nanoscale poly(p-phenylene) (PPP) and zeolites composites for the detection of sulfur dioxide (SO₂) at room temperature. The effects of doping, zeolite types, zeolite contents, and SO₂ concentrations on the relative response and selectivity of the composites were investigated. The sensing response relied upon the doping agent type, doping ratio, and doping temperature which directly affected the electrical conductivity of the material. The sensing selectivity was controlled by zeolite type. Among all conditions, the PPP/ZSM-5 composite with the doping ratio of 50:1, doping temperature of 70 °C, and zeolite content of 30% provided the highest relative response towards SO₂. The composite possessed the sensitivity of 0.0483 ppm⁻¹ with the coefficient of determination (R²) of 0.9927 along with a detection limit of 10 ppm which was determined by the signal to noise ratio. The reversibility of the interaction between the composite and SO₂ was confirmed by the cyclic response. Hereby the sensor based on PPP/ZSM-5 composite is an alternative material to be used in the SO₂ detection.

Abstract ID: 291

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Novel 3D functional architectures consisting of low-dimensional nanomaterials

Keywords: 2D nanomaterials, Nanocomposite, Thermal management, Fire-resistance

“White graphene” and its nanocomposites for thermal management applications

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With the development of technology in civilian and military, high-power density electronic devices are more frequently used than before, resulting in excessive thermal energy accumulation. Therefore, the development of nanomaterials with anisotropic thermal transport properties has attracted increasing attention for thermal management applications, such as coatings in electronics and heat sinks.¹ An ideal candidate should be electrically insulating and have thermal conductivity in-plane significantly greater than through-plane.¹ Two-dimensional (2D) nanomaterials such as graphene and black phosphorus, both of which possess highly anisotropic thermal conductivity, have recently provided a new platform for addressing heat dissipation in devices. However, it is difficult to employ either in thermal management or build components owing to their electrical conductivity and fast oxidation of phosphorus. BN nanosheets offer a high thermal conductivity. In contrast with other conductive and semiconducting 2D materials, BN nanosheets are electrically insulating, which suggests utility in thermal management applications in electronics.²⁻³ Here, we report a free-standing BN nanosheet/polymer composite film with a unique combination of properties including flexibility and toughness, anisotropic thermal conductivity, and fire resistance, which exhibit highly potential applications in high-performance flexible electrically insulating substrates, superior thermal conductivities and fire-resistance coatings.⁴⁻⁹

Key Words: 2D nanomaterials, Nanocomposite, Thermal management, Fire-resistance

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Abstract ID: 292

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Drug delivery/controlled release

Keywords: Magnetite, Nanoparticle, Drug Delivery

Gelatin-coated super paramagnetic nanoparticle for cancer drug delivery

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Drug delivery is the method of administering a pharmaceutical compound to achieve a therapeutic effect on humans based on the drug safety and efficacy at the targeted therapies. The pharmaceutical agents or drugs of interest are entrapped within, or attached to an organic polymer matrix or inorganic particle. Magnetic nanoparticles (MNPs), one of the inorganic nanoparticles, can be manipulated by external magnetic field to lead to the target site. The therapeutic agents are attached to, or encapsulated within, a magnetic nanoparticle by polymer coating. This work aimed to synthesize a magnetite nanoparticle (Fe₃O₄-NP) as a drug carrier via the bio-chemical co-precipitation using a biomaterial template. The cancer drug was attached to the Fe₃O₄-NP through a functional group between the gelatin and the drug. Although, the magnetization of gelatin-coated Fe₃O₄-NP decreased after attaching the drug, the synthesized coated Fe₃O₄-NP possessed the superparamagnetic property. Thus, the gelatin-coated Fe₃O₄-NP was shown to be suitable as a cancer drug carrier as it responded to an external magnetic field and provided suspension stability.

Abstract ID: 293

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Electrostrictive and Magnetostrictive Materials

Keywords: Poly(lactic acid), Carbon nanotube, Actuator

Electro-Responsive Material Based on Multiwall Carbon Nanotube/ Poly(lactic acid) Composites for Using as

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Actuator is a device that is able to change its shape or size under applied external stimuli. The device can be adapted for broad applications such as microelectronic, micro-robotic, and medicine systems. The aim of this work is to develop and fabricate an electrically controlled actuator based on poly (lactic acid) and multiwall carbon nanotube (MWNT) as nano-filler. Dibutyl phthalate (DBP) was used as the plasticizer to reduce the PLA high brittleness. The composites were prepared by solvent casting method. The electromechanical properties of composites were investigated under the effects of graphene concentration and electric field strength. The 0.1%v/v MWNT/PLA/DBP provided the highest storage modulus sensitivity ($\Delta G'/G'0$) of 1.59. Interestingly, the storage modulus response ($\Delta G'$) at the high MWNT concentration of 1.0%v/v became negative in which the storage modulus under applied electric field was lower than the initial storage modulus without electric field. The electric field provided the softening effect. All composites exhibited good recoverability during the temporal response experiments. Thus, these composites can be potentially used as an electroactive material in actuator applications.

Abstract ID: 294 / Poster: 42

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Bio-inorganic nanomaterials

Keywords: Magnetite nanoparticles, biosynthesis, superparamagnetic, mangrove, *Aspergillus*

BIOSYNTHESIS OF MAGNETITE NANOPARTICLES USING *Aspergillus niger* BSC-1 ISOLATED FROM MANGROVE ECOSYSTEM

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Nanotechnology is one of the most promising technologies manipulating materials at nano level. Recently, metal and metal oxide nanoparticles have received a huge attention due to its versatility in every field of science. Synthesis of nanoparticles using biological system is a sustainable and eco-friendly approach. Among the biological systems, fungi isolated from mangrove ecosystem are considered as an excellent source of extracellular bio-active compounds¹. In the present study, iron oxide nanoparticles were synthesized using mangrove fungus *Aspergillus niger* BSC-1 isolated from Indian Sundarban region. The synthesis of nanoparticles was carried out extracellularly by treating fungal cell free extract with inorganic Fe³⁺ and Fe²⁺ salts mixture. UV- VIS spectroscopic analysis of iron salt treated fungal cell free extract exhibited a broad peak at 296 nm wavelength, indicating extracellular synthesis of iron oxide nanoparticles. ATR- FTIR spectroscopy analysis showed peaks at 640 cm⁻¹ and 1635 cm⁻¹, indicating involvement of extracellular protein in synthesis of iron oxide nanoparticles. The measurement of zeta potential determined that the stability of nanoparticles was good as the zeta value was - 32.5 mV. Peaks appeared at 217, 292, 419, 658 cm⁻¹ in Raman spectrum indicated the synthesis of magnetite, which was further confirmed by XRD analysis (JCPDS card No.76-0958). TEM and SEM micrograph of synthesized particles displayed nanoflakes of magnetite with 20-50 nm width, while SAED pattern revealed the crystalline nature and cubic pattern of the magnetite particles. Magnetic property measured by VSM indicated superparamagnetic nature at room temperature. Thus, the present study reported a green and sustainable process for synthesis of magnetic nanoparticles using mangrove fungus.

Abstract ID: 295 / Poster: 12

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Nanocomposites

Keywords: Transparent encapsulation, Organic-inorganic hybrid, Electrochromic

Transparent encapsulation material using methyl-methacryl oligosiloxane nanocomposites for electrochromic devices

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Transparent encapsulation materials are essential for various display applications such as light emitting diodes (LEDs), organic light emitting diodes (OLEDs), and electrochromic devices. For the practical use of the encapsulation materials in those applications, several requirements including high optical transparency and chemical stability, reliable adhesion to the target surface, and ease of fabrication should be addressed.

Organic-inorganic hybrid materials have been widely studied due to their improved physical/chemical properties which originate from the synergistic effects of hybridization of the constituent organic and inorganic components. Sol-gel siloxane hybrid materials are typical organic-inorganic hybrid which exhibits high transparency and chemical stability. However, high volume shrinkage after curing and weak adhesion to the substrate have posed their use in electrochromic application.

For the present study, we fabricated a transparent encapsulation material using methyl-methacryl oligosiloxane resin and colloidal nanosilica. Sol-gel derived methyl-methacryl oligosiloxane resin was synthesized and used as matrix due to its high transparency and chemical robustness. Colloidal nanosilica was also synthesized and reinforced into the matrix resin as nanofiller to reduce volume shrinkage that may give rise to some cracks after curing. Final transparent encapsulation material shows high transparency (>90%), strong adhesion to the substrate (>5B), electrochemical robustness (>10,000 cycles), and solution processability. Physical/chemical property of the encapsulation material and its use in electrochromic devices will be discussed in this presentation.

Abstract ID: 296

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Nano and Environmental catalysis

Keywords: Hybrid catalyst, DNA, Transition metal, Magnetic

DNA based magnetically separable Hybrid Catalysts- Characteristics and Potential Applications

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Hybrid catalysis has emerged as a powerful catalytic concept since over a decade. In hybrid catalysis, a transition metal complex which is catalytically active is anchored to a biopolymer scaffold such as a protein or a polynucleotide to impart enantio-selectivity and increased efficiency to a reaction.

Here we present a novel strategy towards fabrication of DNA based catalysts with its characteristic right-handed helix structure containing a transition metal complex as well as magnetic iron oxide that makes the catalyst magnetically separable.

Iron (II,III) oxide Fe₃O₄ nanoparticles are grafted with diethylenetriamine pentaacetic acid (IO-DTPA) through non covalent interactions. The polyaminocarboxylic acid -functionalized nanoparticles, IO-DTPA NPs were further used to bind DNA molecules. The formation of IO-DTPA NPs of size 5-20 nm was confirmed by X-Ray diffraction (XRD), Infrared Spectroscopy (IR), Ultraviolet (UV) spectroscopy and magnetization studies. Infrared spectroscopy, further allowed to identify the carboxyl and amino functional groups on the surface of the nanoparticles. The IO-DTPA NPs were further bound to transition metals and DNA through the polyamino carboxylic groups of DTPA to give a magnetic DNA transition metal hybrid catalyst (DNA-TM). The unique characteristics and potential applications of DNA-TM will be discussed.

Abstract ID: 297

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: Triboelectricity, Piezoelectricity, Hybrid Nanogenerator, Renewable Energy, Sensor, Transducer

Li-ZnO Nanowire/Polymer Nanocomposite Based Piezo-Tribo Hybrid Nanogenerator

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With the robust development of piezoelectric and triboelectric nanogenerator, hybrid nanogenerator is passing its golden moments of improvements. Here we demonstrate a novel, unpoled and cost-effective piezoelectric-triboelectric device structure to enhance the electrical conversion of electromechanical action. Piezoelectric film was constructed using Lithium Doped Zinc Oxide (Li-ZnO) Nanowires (NWs) and Multiwalled Carbon Nanotubes (MWCNTs) in Polyvinylidene fluoride (PVDF) polymer matrix. PEG coating on Li-ZnO NW worked as a surface modification and enhanced β phase formation in Polyvinylidene fluoride (PVDF) polymer. The triboelectric layer was constructed using Polydimethylsiloxane (PDMS)-Polytetrafluoroethylene (PTFE) copolymer on flexible Aluminium foil. PTFE spacer was utilized in between piezoelectric, triboelectric layers. The hybrid nanogenerator was later tested with different loading conditions and found a promising response. Maximum output was found to be potential of 60.1V and short circuit current of 75 μ A. Because of nanocomposites, the nanogenerator produced a continuous surge of electricity as a response towards the constant a load. Piezoelectric and triboelectric nanogenerator demonstrated their distinctive character in generated response. Hence it can be a real life superior power generation device and a self-powered transducer.

Abstract ID: 298 / Poster: 11

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Nanocomposites

Keywords: Transparent encapsulation, Organo siloxane, Optoelectronic device

Transparent, thixotropic, and adhesive encapsulation for optoelectronic devices

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With the increasing development of optoelectronic devices such as organic light emitting diodes (OLEDs) and organic photovoltaic devices (OPVs), optically transparent and chemically robust encapsulation materials have attracted great attention due to the fact that the effective protection of such devices is of crucial importance.

Organo siloxane compounds are most widely used encapsulation materials for LEDs and other display devices. The barely-existing carbon-carbon bonds and their high temperatures of decomposition that stems from strong silicon-oxygen bonds, compared to usual organic polymers, made these materials popular. In addition, ease of synthesis protocol, which lies on simple sol-gel process, makes this material well suit for commercial availability.

In this presentation, we synthesized sol-gel derived organo siloxane (OS) resins which can be used as high performance encapsulation materials for various optoelectronic device applications such as displays and photovoltaics. The OS resins are synthesized using several organo silane precursors via hydrolytic or non-hydrolytic sol-gel process. The as-synthesized OS resins have high optical transparency, high temperature stability, enduring chemical stability and adhesive property. To provide both thixotropic property and adjustable viscosity, functional additives are put into the OS resins. Then, the final encapsulation materials can be used in low-cost solution processing such as screen-printing and nozzle-printing.

Thursday, 22/Aug/2019 9:06am - 9:18am

Abstract ID: 299 / FCM-2: 6

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Failure of Composites

Keywords: XFEM, debonding, cohesive model

Modeling of short fiber reinforced composite using Extended Finite Element Method (XFEM)

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The short-flax-fiber-reinforced polymer composites usage is increasing for various engineering applications such as automobile industry. With the increasing demand of these composites, it is needed to predict mechanical and failure behavior using simulations. The aim of present work is computational investigations to find the mechanical and failure behavior of short-flax-fiber-reinforced polypropylene composite within the XFEM framework. In the computational model, polypropylene matrix and flax fiber deformation will be considered as elasto-plastic and elastic manner respectively. The modeling strategy will be developed for very high aspect ratio inclusions. The progressive debonding between the fiber and the matrix will be modeled by prescribing cohesive zone laws. The uniform distribution of inclusions in the matrix will be considered. With the application of tensile load, the computational study will be conducted for representative volume element.

The fiber-matrix deboning is assumed to be initiated by fiber inclusions and continuum damage approached is to be used for matrix cracking. The multi inclusions crack interaction behavior will be studied at different fiber orientation. The simulation results will be obtained in the form of stress and strain curve. The developed simulation model will be validated with experimental results. Presently the processing of composite is underway.

Abstract ID: 300

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Plasma-Surface Interactions for Thin Film Engineering

Keywords: Surface plasmon, Optical trapping force, Composite Metallic Film

A Numerical Study about Optical Trapping Properties of Nanoparticle on Composite Metallic Film

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Recent years, optical trapping and manipulation of particles have been widely used in different areas of science particularly in researching the optical trapping properties of surface plasmon polaritons(SPPs) due to the advantages of being high precision and sensitivity[1], since the pioneering work of Ashkin et al. on trapping a dielectric microsphere using a single focused laser beam. Nowadays it has been applied to manipulate nanoparticle near the composite metallic film with periodic structure.

Based on the three-dimensional dispersive finite difference time domain(FDTD) method and Maxwell stress tensor equation, the optical trapping properties of nanoparticle placed on the composite metallic film are investigated numerically. Surface plasmon polaritons are excited on the metal-dielectric interface with particular emphasis on the crucial role in tailoring the optical force acting on a nearby nanoparticle. In order to obtain the detailed trapping properties of nanoparticle, selected calculations on the effects of beam waist radius, sizes of nanoparticle and circular holes, distance between incident Gaussian beam and composite metallic film, material of nanoparticle and polarization angles of incident wave are analyzed in detail to demonstrate that the optical trapping force can be interpreted as a virtual spring which has a restoring force to perform positive and negative forces as nanoparticle moving closer to or away from the centers of periodic structure. The results could provide guidelines for further research on the optical system design and manipulation of arbitrary composite nanoparticles.

Abstract ID: 301

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Computational studies of Biomaterials

Keywords: Bessel beams; Lateral binding force; chiral spheres

Stability and dynamics of self-arranged chiral structures in lateral optical binding

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The Generalized Lorenz Mie theory and the Foldy-Lax multiple-scattering equations are applied to compute the lateral binding force (BF) of an arbitrary number of chiral spheres of arbitrary size, subject to Bessel beam incidence. Such non-diffracting light suppressed the influence of the axial intensity profile of the illuminating beams on the self-organization process which then depended critically upon the inter-particles interactions. The theory and codes for lateral binding force are verified when the chiral spheres degenerates into isotropic spheres. We discuss the influence of the particle number, permittivity, and chirality parameter in detail. Linearly and circularly polarized incident Bessel beams are considered, and the corresponding binding forces are compared and analyzed. It is shown that the lateral binding force between chiral spheres can be significantly discriminatory in nature, depending upon both the handedness of the interacting particles and the polarization of the incident light. In binding chiral spheres, therefore, the polarization of incident beams should be chosen in accordance with the chirality. This finding may provide a recipe to understand the light interaction with multiple chiral particles of arbitrary shapes (in general) with the aid of the analytical approach. It could be a promising avenue in controlling the optical micromanipulation on chiral structures self-arrangement.

Abstract ID: 302

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Computational studies of Biomaterials

Keywords: High-order Bessel beam; Optical binding; Multi-layered biological cells

Interactions between stratified biological cells optically trapped in high-order Bessel beams

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Based on the generalized multi-particle Mie equation (GMM) and Electromagnetic Momentum (EM) theory, the interactional scattering and optical binding between stratified biological cells induced by an arbitrary polarized high-order Bessel beam (HOBB) are investigated with particular emphasis on the half-conical angle of the wave number components. The illuminating HOBB is described in terms of beam shape coefficients (BSCs) within the framework of generalized Lorenz-Mie theories (GLMT). Different types of cells, including a real Chinese Hamster Ovary (CHO) cell and a lymphocyte which are respectively modeled by a coated and five-layered sphere, are studied. Numerical effects of various parameters such as beam polarization angles, incident wavelengths, particle sizes are numerically analyzed in detail. The observed dependence of the separation of optically bound particles on the incidence of HOBB is in agreement with earlier theoretical prediction. Accurate investigation of interactions induced by HOBB could provide an effective test for further research on optical binding between more complex biological particles, which plays an important role in using optical manipulation on particle self-assembly.

The geometry of two multi-layered spheres illuminated by a first-order Bessel beam with arbitrary direction is given in Fig. 1(a). Fig. 1(b) shows optical binding force of lymphocyte cells for different beam conical angles induced by a first-order Bessel beam. The lymphocytes are modeled by a five-layered sphere [1]. The corresponding binding spring constants with regard to small conical angles are larger than those of large conical angles, especially for the first and second stable equilibrium positions. The authors do further research on BF between more complex stratified biological bi-sphere in this paper.

Abstract ID: 303 / Poster: 31

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Carbon/Carbon Composites

Keywords: Thermal insulator, SiC, Coating, Oxidation resistance, carbon fiber composites

SiC-conversion coating prepared from silica sol for improving oxidation resistance of carbon-fiber composites

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Carbon fibers, which have excellent mechanical and thermal properties, are used in many field, but they are very vulnerable to oxidation and have limited service life. Various studies have been conducted to solve this problem. In this study a SiC–C composite material was prepared by using a silica sol to coat the carbon surface and improve the oxidation resistance of a carbon-fiber insulator as a material for solar-cell ingot-growing crucibles. The SiC coating was formed on the carbon surface under various conditions by controlling the composition of the silica sol, and its characteristics were examined. As a result of the SiC-conversion coating process through a carbothermal reaction, a film with thickness of 30–80 nm thick film was uniformly formed over the entire sample. In addition, the oxidation characteristics were enhanced by a factor of three to five when compared with conventional carbon materials. Also, there is no change in thermal conductivity after coating using a silica sol.

Abstract ID: 304

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Poster Presentation

Topics: Fuel Cells

Keywords: Solid Oxide Fuel Cells, Cathode, Electrodeposition, Perovskite

High-performance nanofibrous LaCoO₃ perovskite cathode for solid oxide fuel cells fabricated via chemically assisted electrodeposition

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A new method is developed for the fabrication of nanofibrous LaCoO₃ (LCO) perovskites as cathodes (oxygen electrodes) for solid oxide fuel cells (SOFCs). The proposed method involves chemically assisted electrodeposition (CAED) of mixed metal hydroxide onto a carbon nanotube (CNT) template, followed by a low-temperature heat-treatment process. The CNT template is first fabricated on porous zirconia-based ion-conducting scaffolds (ICS) by catalytic chemical vapor deposition (CCVD) of C₂H₄. Perovskite-type LCO is then fabricated on the CNT template by CAED process of mixed La–Co hydroxide combined with thermal conversion of hydroxide to perovskite oxide. The method proposed here allows for the fabrication of LCO perovskites with a unique nanofibrous structure at reduced temperatures (□900 oC), while avoiding the formation of pyrochlore phases (e.g., La₂Zr₂O₇), which are typically observed during conventional high-temperature sintering processes of LaCoO₃ with zirconia-based electrolytes. The new method also provides the precise control needed to achieve desired oxide loadings without the need for repeated deposition-annealing processes. The anode-supported SOFCs with nanofibrous LCO cathodes on zirconia and ceria scaffolds show high and stable electrochemical performance of 0.95 and 1.27 W cm⁻², respectively, at 800 oC. In addition to the absence of insulating pyrochlore phases, the unique nanostructure of the LCO cathode is believed to play a beneficial role in improving the electrochemical properties by providing a large number of active reaction sites and by facilitating mass transport through the porous nanofibrous structure.

Abstract ID: 305

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Optical, Optoelectronic and Dielectric Coatings

Keywords: solar-thermal conversion, solar selective absorber, metal/dielectric multilayered film structure

High efficient and thermally stable solar selective absorbers based on multi-layered metal/dielectric film structure

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As one of the most prevalent solar energy utilization technologies, solar-thermal conversion can harvest most part of the incident solar photons, with practical applications such as solar heating, solar-thermal-electricity, solar-thermoelectrics, solar-thermophotovoltaics, and so on. In solar-thermal conversion process, solar selective absorber is the most crucial component to absorb the most part of the solar radiation in a broad wavelength region, while surpass the infrared re-radiation to reduce the heat loss.

In this work, a series of metal/dielectric multilayered solar absorbers was designed and fabricated. (1) To improve thermal stability, an atomic-layer-deposited Al₂O₃ barrier layer was adopted to improve the thermal stability of the multilayered film structure; (2) To keep the layer numbers as few as possible, nano-composite, alloy or textured surface was introduced into the multilayered design, respectively.

Thursday, 22/Aug/2019 10:24am - 10:36am

Abstract ID: 306 / FESC: 13

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Fuel Cells

Keywords: Graphene, Microfluidic fuel cell, fuel breathing, porous electrode

Fuel Breathing Microfluidic fuel cell: fuel solubility effect to the anode selection

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Microfluidic fuel cell (MFC) is a promising solution to achieve a sustainable future. Different catalysts and the electrode structure were developed and engineered for different fuel oxidation process. The matching of fuel and catalyst was well established in the literature and it was shown that the flow through porous electrode which provided larger reactive area was beneficial to the fuel oxidation when fuel was provided in liquid form[1]. However, the effect of electrode structure to different fuels in the vapour feed microfluidic fuel cell has yet to be studied. A 3D anode with PtRu nanoparticles on graphene aerogel is synthesized and a microfluidic fuel cell is designed to test and compare the performance with commercial 2D anode. The PtRu nanoparticles are about 3 nm and evenly decorated on the graphene nanosheets. The methanol breathing MFC with 3D anode has nearly a doubled peak power output comparing with its 2D counterpart. However, the hydrogen breathing MFC performs excellently with the 2D anode while the peak power drops dramatically with the 3D anode. This suggests that matching fuel solubility with electrode structure is also important for selecting the anode for fuel breathing microfluidic fuel cells.

References

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Abstract ID: 307

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Ceramic based composites

Keywords: saucer structure, graphene aerogels, porous graphene aerogels -oxide ceramics, ultralow thermal conductivity, spark plasma sintering

Ultralow thermal conductivity in graphene- oxide porous ceramics with special saucer structure of graphene aerogels

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In our work, a unique saucer structure of graphene aerogels in the form of large-size graphene sheets is designed to be direct grown in situ on hollow oxide (silica, zirconia, alumina) spheres that are connected to their neighbors by C-O and C-Si (C-Zr, C-Al) bonds after fabrication by spark plasma sintering (SPS). The porous graphene -oxide (silica, zirconia, alumina) ceramics are characterized by Fourier transform infrared (FTIR), Raman and X-ray photoelectron (XPS) spectroscopies. The mechanism of metal-catalyst-free method for the direct synthesis of graphene aerogels in the form of large-size graphene sheets on hollow spheres is studied. Compared to other ceramics, porous ceramics have an ultralow thermal conductivity and a relatively high compressive strength, which depends on the special saucer structure of graphene aerogels and high porosity. The temperature dependence of the thermal conductivity is altered by the content of graphene aerogels.

Abstract ID: 308

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Electrochemical Supercapacitors

Keywords: Energy storage, Electrochemical properties, Supercapacitors

Fabrication of Zn_{1-x}Cu_xCo₂O₄ nanostructured based High-Performance symmetric supercapacitors

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High-performance and environmentally friendly energy storage devices, such as supercapacitors are urgently needed for sustainable and renewable power sources in modern electronic industry. ZnCo₂O₄ is a promising functional material that has been investigated as electrodes for high performance supercapacitors.

In this work, Cu Substituted ZnCo₂O₄ rods were synthesized by simple hydrothermal approach. Structural and morphological properties of pure and Cu-Substituted ZnCo₂O₄ have been characterized by X-ray diffraction (XRD), energy-dispersive X-ray spectrometer (EDX), scanning electron microscope and high-resolution transmission electron microscopy. XRD data confirm the pure phase formation of samples. Electron microscopic studies show the rods morphology of Zn_{0.7}Cu_{0.3}Co₂O₄. The Brunauer–Emmett–Teller (BET) specific surface area of Zn_{0.7}Cu_{0.3}Co₂O₄ rods is found to be 52 m²g⁻¹ with an average pore size distribution of 9 nm. The electrochemical properties of the samples were studied by cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD) measurement in three-electrode configuration with 6M KOH as the electrolyte. Zn_{0.7}Cu_{0.3}Co₂O₄ exhibits maximum specific capacitance of 1425 Fg⁻¹ at a current density of 1 Ag⁻¹. Besides, 95% of specific capacitance is retained for 2000 cycling stability of Zn_{0.7}Cu_{0.3}Co₂O₄ rods, examined by GCD measurements. The results indicate that the Zn_{0.7}Cu_{0.3}Co₂O₄ is a potential material for SCs. Further, symmetric SCs are assembled to achieve high energy density with superior cyclic stability.

Key Words: Energy storage, Electrochemical properties, Supercapacitors.

References

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Abstract ID: 309

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: 3D Scaffolds

Keywords: Breast tumor model, Decellularized lung matrix, Chitosan/gelatin, Poly-L-lactic acid, Drug resistance

Comparison and evaluation of tissue-engineered 3D tumor model based on different resources of biomaterials

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Potential anti-cancer drugs are commonly of low efficacy in clinics due to the lack of predictive models or the insufficient employment of existing preclinical test systems. Three-dimensional (3D) in vitro engineered tumor models can better predict the efficacy of novel drugs by reproducing the in vivo tumor microenvironment. In this study, three derived scaffolds (decellularized lung scaffold, chitosan/gelatin scaffold, and poly-L-lactic acid scaffold) incorporated with breast cancer cells (MCF-7, 4T1) were bioengineered as a platform for in vitro solid tumor development. The good biocompatibility of three scaffolds favored cell growth and proliferation. Cells in 3D scaffolds were less sensitive to chemotherapy and displayed characteristics of higher malignancy as compared to those in 2D cultures. Interestingly, MCF-7 cells cultured in three scaffolds exhibited similar growth pattern, while 4T1 cells grew into denser tumor spheroids in the chitosan/gelatin scaffold. The expression of breast cancer biomarkers in MCF-7 cells significantly increased in 3D scaffolds compared to their 2D counterparts. Cells grown in 3D scaffolds were found to be more tumorigenic and angiogenic in BALB/c mice xenografts than cells grown from monolayers. The results demonstrate that 3D engineered tumor model is a better representative of the in vivo tumor and can serve as a more effective platform for the study and screening of novel cancer therapeutics.

Abstract ID: 310

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Theory of Structure, Surface and Interface of thin films

Keywords: super-amphiphobic, TiO₂, super-hydrophilic, coating, oil-water separation

A novel functional thin film based on black TiO₂: super-amphiphobic surface transfer to super-hydrophilic/super-oleophobic surface via nature light activation

Hong ZHONG¹, Yuanhao WANG², Lin LU¹

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Low cost super-amphiphobic coating is promising film material for future membrane application. TiO₂ has been attracting much interests in surface science, due to its high performance in super-hydrophilic after light activation and its low cost in mass production. In this study, a novel super-amphiphobic coating based on black TiO₂ has been newly developed and investigated. Through the emulsion template, the special porous microstructure of SiO₂ has been obtained. Then, anatase TiO₂ would be covered on the surface of SiO₂ with the controllable hydrothermal reaction. After optimized electroreduction experiment, the anatase TiO₂ would be transferred to black TiO₂ which is mainly composed of self-doped TiO₂. A portion of Ti⁴⁺ ions is reduced to Ti³⁺, and then the oxygen vacancies are passively protected. The final film exhibited an outstanding super-amphiphobic performance, and both drop contact of water droplet and 1,2-dichloroethane were higher than 150°. After nature light activating, the water contact angle would decrease. After 30 minutes' sunlight radiation, the surface showed an amazing super-hydrophilic performance, which results in a low water contact angle of lower than 10°, while the drop contact angle of 1,2-dichloroethane was still higher than 150°. The results prove that the novel coating is robust and multifunctional with potential applications of self-cleaning, oil-water separation, and extraction. Furthermore, the super-amphiphobic coatings based on other photocatalysis materials can be developed through this novel process method.

Abstract ID: 311

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Aqueous lithium ion batteries

Keywords: Aqueous Battery, Energy Storage, Proton Insertion, Electrochemistry

Investigating coupled Electron-Proton storage at mesoporous metal oxide films under mild aqueous conditions

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There is currently strong societal demand for the development of rechargeable batteries that meet stringent criteria in terms of cost, safety, toxicity and ecological impact, particularly for scalable grid storage systems required by the development of renewable but intermittent energy sources.¹ This has led to a renewed interest in neutral aqueous electrolytes with high ionic conductivity, especially since recent studies demonstrate that the main limitation related to the low electrochemical thermodynamic stability window of water could be overcome by the use of water-in-salt electrolytes.² This has also led to search for aqueous intercalation-type electrodes beyond Li-ion, which geo-availability, cost and aqueous solubility are problematic issues.³

In this context, we investigated the ability of the proton-ion, i.e. H⁺, to insert reversibly within mesoporous metal oxide electrodes such as TiO₂ upon reductive electrochemical conditions. We demonstrated that coupled electron-proton storage occurs not only under strong acidic conditions, but more interestingly also under neutral pH conditions in presence of a weak acid.⁴ The process was modeled by a three-step mechanism, which allowed determining the solid-state diffusion coefficient of proton within the metal oxide lattice. More recently, we have demonstrated that coupled electron-proton charge storage at mesoporous metal oxide electrodes can be generalized to a wide range of organic as well as inorganic weak acids, and to other electrode materials than TiO₂. Accordingly, this study paves the way for the development of low-cost and eco-friendly rechargeable aqueous battery entirely based on proton-ion intercalation and characterized by improved charging rates and cyclability thanks to its small ionic radius.

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Abstract ID: 312

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Polymeric composites

Keywords: Humidity Sensor, Polymer, Composite, Thin Film

Characterization of coplanar capacitive type humidity sensor fabricated using a composite thin film of PTB7-Th:VOPcPhO

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In the present work, a capacitive humidity sensor is fabricated using a composite thin film of poly[4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b;4,5-b']dithiophene-2,6-diyl-alt-(4-(2-ethylhexyl)-3-fluorothieno[3,4-b]thiophene-)-2-carboxylate-2-6-diyl] (PTB7-Th) and Vanadyl 2,9,16,23-tetraphenoxy-29H,31H-phthalocyanine (VOPcPhO) on aluminum coplanar electrodes. The sensor with a concentration of PTB7-Th: VOPcPhO ~ 2:1 exhibits better sensitivity and linearity and fast response time. The device shows sensitivity over a large range of relative humidity levels (between 20 and 95 % RH). Typical adsorption and desorption response times were measured to be 5 and 6 s respectively.

Abstract ID: 313**Symposium 1: Functional Biomaterials and Biosensors (FBB)****Poster Presentation**

Topics: Bio-inorganic nanomaterials

Keywords: Manglicolous Fungi, Iron oxide nanoparticle, waste water, Indian Sunderban

Adsorption of Cr(VI) from synthetic industrial waste water by iron oxide nanoparticles synthesized using manglicolous fungi isolated from Indian Sunderbans

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Water pollution due to industrial waste water is one of the major concerns of recent era which is affecting the human and animal lives in all aspects. Thus, the management of industrial waste water is an essential critical topic. In the present study synthesis of iron oxide nanoparticles was done using manglicolous fungi isolated from Indian Sunderbans which then utilized for the removal of Cr(VI) from synthetic industrial waste water. 15 fungi were isolated from coastal mangrove sediment of Sathjelia Island area located in Indian Sunderban. Fungal Cell filtrate (FCF) of these 15 fungi was screened to identify their potentiality to hydrolyze the mixture of FeCl₂ and FeCl₃ salts for the production of iron oxide nanoparticles. One isolate (STSP19) had shown positive result. This isolate was morphologically identified as *Phialemoniopsis* sp. The extracellular bio-reduction can be observed by changes in the colour of FCF which was monitored by analysing the reaction mixture in UV-Vis Spectrophotometer. The bio-synthesized particles were characterised by Fourier transform infrared (FTIR) spectroscopy to understand the involvement of fungal proteins with iron-nanoparticle. The stability of iron-nanoparticle was confirmed by measuring the Zeta Potential of the iron-nanoparticle solution. The iron-nanoparticle were found to be spherical with average particle size ranging between 5-10 nm were confirmed by Field Emission Scanning Electron Microscopy (FESEM) and Transmission Electron Microscopy (TEM). Energy Dispersive spectroscopy (EDS) analysis was performed during FESEM study to confirm the presence of elemental Fe in the sample. Selected Area Electron Diffraction (SAED) and X-Ray Diffraction (XRD) pattern confirms the nature of green synthesized iron-nanoparticles. Both studies was carried out for the removal of Cr(VI) in different experimental conditions like pH (2-10), contact time (15-120 min), adsorbent dose (0.1-0.3 g/L) and temperature (293-313 K). The data recorded were subjected to different isotherm and kinetic model. Temkin isotherm and Pseudo second order was found to be best fitted model. Adsorption of Cr(VI) from waste water on iron oxide nanoparticles was chemisorption in nature with maximum adsorption capacity of 17.857mg/g. Green synthesized iron oxide nanoparticle thus is an effective tool for water treatment.

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Abstract ID: 314

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Environmental biosensors

Keywords: sensing, nanoparticles, Chitosan

Green receptor based qualitative estimation of mercury detection in aqueous solution

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Impregnating optical waveguides with suitable functional elements have enabled copious qualitative as well as quantitative sensing procedures. However, in most cases, the interaction procedure is activated through non green route. Entailing green route is promising as well as challenging task. Herein, we developed a green approach towards sensing mercury, a pervasive environmental pollutant toxic approach. The proposed scheme, entailing a biodegradable polymer Chitosan as functional element, has been proven to be highly functional and cost-effective as compared to other existing approaches. Impregnating Chitosan functionalized Ag nanoparticles onto a U shaped fiber optic probe, we have shown excellent selectivity of this heavy metal ion in aqueous solution amongst others. Based entirely on intensity modulation, this green approach based scheme is found to possess superior sensitivity. This study renders a promising route to greatly enhance the sensing properties of optical waveguides through suitable functional elements and provides suggestive insights for developing high-performance real time monitoring unit.

Abstract ID: 315

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

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

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

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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 nanorods have photothermal properties at ~808 nm because 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 $\lambda = 808$ 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.

Abstract ID: 316

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Composites in Innovative Applications

Keywords: Atrazine; herbicide; iron composite; water.

Adsorption, kinetics and thermodynamics studies of removal of atrazine herbicide using composite nanomaterials

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The organic pollutant, namely Atrazine has been found in several water resources of the world. It is highly toxic and carcinogenic in nature. Atrazine is removed by adsorption on iron composite nanoparticles. The composite nanoparticles were synthesized, analyzed and applied for atrazine uptake from water. Residual atrazine was monitored by gas chromatography–mass spectrometry. The maximum atrazine removal (95 %) was achieved using contact time 30 min, concentration 30 µg/L, pH 7, dose 2.5 g/L and temperature 20 °C. The adsorbent was selective for atrazine adsorption. The results obeyed Langmuir, Freundlich, Temkin and Dubinin–Radushkevich isotherms. ΔG° values were -6.05 , -6.11 and -6.15 kJ/mol at 20, 25 and 30 °C temperatures, respectively. The value of ΔS° was -2.45×10^{-3} kJ/mol K. It showed decline in entropy of atrazine uptake. The adsorption followed pseudo-second-order kinetics. The adsorption mechanism was liquid film diffusion. The proposed adsorption method is inexpensive, fast and reproducible. It can be used to remove atrazine from any water sample/source.

Abstract ID: 317

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Dielectric, Ferroelectric and Piezoelectric materials

Keywords: Density Functional Theory, Ground State, Orthorhombic, Ferromagnetic

First principles calculation of the structure and magnetic ordering in ErF₃

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Erbium is one of the 14 earth elements and belong to the family of lanthanides. Erbium is alloyed with a number of metals for different uses. Erbium can also be mixed with inorganic minerals such as fluoride to form erbium fluoride. Fluorides are abundantly available in nature and are also known to be alloyed to metals. Erbium has application in the military and in telecommunication but is quite costly. The use of erbium fluoride is predominant in pharmaceuticals. Understanding properties of erbium fluoride at ground state may reveal other promising application of the material especially as functional material. The orthorhombic atomic structure of erbium trifluoride was investigated using a first principles molecular dynamics (FPMD) simulation based on density-functional theory (DFT) calculations. The results demonstrate that ferromagnetic ordering of the Er moments is energetically confirmed when compared to the experimental data obtained via magnetic neutron diffraction experiments. Er t_{2g} states, which are responsible for the magnetism, have only a very small interaction with F e_g states, which results in a small exchange splitting of these states.

Thursday, 22/Aug/2019 2:15pm - 2:27pm

Abstract ID: 318 / FLNM-3: 2

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Photonic and optoelectronic device applications of low dimensional, nano and 2D materials

Keywords: Graphene, Up-conversion nanoparticles, Fluorescence Quenching and Enhancement, Hybrid photodetector, Responsivity.

High responsivity broadband photo detection by graphene engineered core, and core-shell upconversion nanoparticles

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Hybrid graphene-upconversion nanoparticles (UCNP) photodetectors have recently attracted much interest due to its range of applications in bio-imaging, FRET based bio-sensor, cancer therapy, anti-counterfeiting, NIR wave guide, and in solar cells. UCNPs have unique energy sublevels constituting inner 4f–4f orbital electronic transitions, longer excited state life time (millisecond), NIR excitation and visible emission, which make these nanoparticles suit these applications[1]. Recently, these UCNPs have shown promise as photodetectors requiring a charge transport layer, such as graphene, for carrier collection. Most of the UCNP based photodetectors have very low response and complicated active core-shell structure and are based on fluorescence quenching[2]. In this work we have fabricated graphene-UCNP composite devices, based on both fluorescence quenching (for core UCNPs) and fluorescence enhancement (for silica coated core-shell SiO₂@UCNPs) and found that the latter device has a significant enhancement in responsivity as compared to the former. The responsivity of the core-shell based device is nearly double, 2×10^3 AW⁻¹, that of the core device. This is much higher than the previously reported responsivity observed in UCNP and graphene based devices. Furthermore, we have studied the detection capability of the device in response to various domestic appliances, such as, laser pointers, cellphone flash light, and air-condition remote controllers and found it working efficiently. This work will provide new directions to the ongoing materials research for high sensitivity photo detection.

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Thursday, 22/Aug/2019 11:12am - 11:24am

Abstract ID: 319 / FCM-3: 2

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: Molybdenum disulphide, Upconversion nanoparticles, Nanocomposites, Photodetector, Broadband, Responsivity

Ultrasensitive broadband photodetector using electrostatically conjugated MoS₂-upconversion nanoparticles nanocomposite

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Recently, hybrid or composite nanomaterials have gained a lot of attention due to their interfacial properties, especially showing strikingly different, or even extended optoelectronic performance over individual nanomaterial [1,2]. Conjugating the right materials to generate the desired properties is the key to such applications. In this work, we have synthesized a novel electrostatically conjugated nanocomposite material containing 2-Dimensional MoS₂ nanoflakes and a multi-photon absorbing phosphor, lanthanide doped upconversion nanoparticles (UCNPs), to make a broadband photodetector that has shown responsivity, and gain surpassing the best reported till date by at least an order of magnitude. The device, prepared by electrostatic conjugation of the materials, and Au/Pt contacts drawn by focused ion beam, was studied under a range of wavelengths with variable powers. A highest photoresponsivity of 1254 A W⁻¹ is obtained for 980 nm at 1 V bias and a lowest responsivity of 81 A W⁻¹ is obtained of 808 nm at 0.1V bias. The broadband nature of photoabsorption was attributed to the few layer MoS₂, and the extension of the photoresponse in the infrared was attributed to the UCNPs that had 980 nm absorption. Plotting the photoresponsivity of the nanocomposite, as a function of the wavelength we demonstrate that follows the trend of convoluted optical absorption of the individual components in the nanocomposite. This novel and high responsivity nanocomposite material is the next-generation photodetector.

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Abstract ID: 320

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Structural, Electronic, Optical and Magnetic Properties

Keywords: Density Functional Theory, Structural Properties, Electronic Properties

A castep study of TbBr₃ structural and electronic properties

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Terbium is a chemical element found in many minerals. It is used to dope materials that are used in solid-state devices, as a crystal stabilizer of fuel cells which operate at elevated temperatures. It also finds use in actuators, in naval sonar systems and in sensors. On the other hand, metal bromide compounds which are water soluble find usage in water treatment, chemical analysis and in ultra high purity for certain crystal growth applications. The binary semiconductor terbium bromide (TbBr₃) is studied by using the first-principles methods in the density functional theory (DFT) framework. The structural and electronic properties were calculated at the ambient pressures in the generalized gradient and local density approximations. The structural properties are determined to be closer to those found experimentally. The compound was shown to have an indirect band gap of about 1.742/1.889 eV in both approximations. The obtained results, which are reported, can facilitate assessment of possible applications in sensors and biosensors.

Abstract ID: 321 / Poster: 45

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Ceramic based composites

Keywords: Superconducting composite, Nano, Electromagnetic property

Electromagnetic properties of YBCO superconducting composite for magnet application

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In order to put superconducting materials to practical use in energy, mechanical, transportation, medical, and electronic industries, it is necessary to improve the characteristics of superconducting transition temperatures and the critical current density of superconducting materials. Techniques should be developed for processing shapes such as wire or bulk, which are suitable for specific application. The magnetic properties of superconductors derived from this study show that the physical properties of superconducting specimens with top seeding growth and interior seeding are significantly improved compared to interior seeding superconducting samples. The results of the FC measurement, which is the method of measuring the maximum attraction force, are similar to those of the previous ZFC measurement. The upper surface of the superconducting specimen is composed of a specimen made by the interior seeding method with a large growth of a-c sector, As a result of the top + interior seeding method, the results of the top + interior seeding method showed about 10 N higher values. This result shows that the growth rate of the a-b sector, which improves the magnetic properties of the superconducting specimen, is higher when two seeds are used. This research was supported by the Korean Electric Power Corporation [Grant number:R16XA01]

Wednesday, 21/Aug/2019 4:12pm - 4:24pm

Abstract ID: 322 / FCM: 2

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Shape-memory alloy

Keywords: Ferromagnetic Shape Memory Alloys, Multifunctional alloys, NiMnGa

Microstructure, magnetic behavior and nanomechanical characterization of NiMnGa-based multifunctional ferromagnetic shape memory alloys

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Shape Memory Materials (SMM) and especially ferromagnetic shape memory alloys (FSMA) are nowadays one of the most promising group of modern smart materials [1]. They attract considerable attention of numerous research groups due to their complex multifunctional behavior. In a view of potential application, the existence of thermally, magnetically and stress induced reversible martensitic transitions in these types of materials contributes to many desirable properties, including shape memory effect, magnetic field induced strains, superelasticity, large magnetoresistance, exchange bias as well as magneto- and mechano-caloric effects [2]. In this work the effect of Ti and Gd addition on microstructure, martensitic transformation temperatures, magnetic and mechanical properties of the Ni₅₀Mn₂₅Ga₂₀X₅ (X=Ti or Gd) alloy is in detail investigated. Microstructural studies performed by Scanning Electron Microscope and X-Ray Diffractometer revealed a single phase structure in Ti-doped alloy, whereas a dual-phase structure in Gd-doped alloy was observed. Topography investigations conducted on Atomic Force Microscope helped to discover and characterize the periodic martensitic laths in the Ni₅₀Mn₂₅Ga₂₀Gd₅ sample. Magnetic properties and phase transformation temperatures were investigated with the help of Vibrating Sample Magnetometer (VSM) at wide range of temperatures from 50 to 400 K and external magnetic field up to 3 T. These measurements shown the strong correlation between chemical composition of the alloys and their magnetostructural behavior. Nanomechanical characterization of the prepared materials were done with the help of Nanoindentation Tester. The series of instrumented nanoindentation performed in a form of square grid allowed to determine the mechanical properties, such as hardness, elastic modulus and deformation energy of the single phase Ni₅₀Mn₂₅Ga₂₀Ti₅ alloy and each individual phase of the dual-phase Ni₅₀Mn₂₅Ga₂₀Gd₅ alloy. Collected nanoindentation data were also used to prepare the visual surface distribution of mechanical properties. The presented studies provide a significant contribution for the development of multifunctional ferromagnetic shape memory alloys.

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Abstract ID: 323

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Photocatalytic and electrochemical water splitting

Keywords: CdSe, TiO₂, photoanode, water-splitting

Mushroom-like structural CdSe/TiO₂ Heteronanorods for enhancing light absorption and application in photoelectrochemical cell

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The photocatalytic decomposition of water is believed to be able to help mitigate the crisis of fossil fuel depletion. However, the photocatalytic hydrogen production remains challenge to obtain high photoconversion efficiency. Tailoring the nano-morphology and nano-architecture of photoanode is the most important approach to design high photocatalytic activity photoanode for hydrogen evolution. Here we report a mushroom-like structural CdSe/TiO₂ as efficient photoanodes via simple room-temperature, low-cost electrochemical deposition. The microstructure and composition of the CdSe top layer are regulated and controlled by electrochemical deposition current density and the deposition amount of CdSe. The results show that one-dimensional mushroom-like structural CdSe/TiO₂ (CdSe nano-sphere grow on the top ending of CdSe/TiO₂ nanorods) perform enhancing the photocatalytic ability because of the CdSe nano-sphere heighten the absorption of light. Besides, with the increasing deposition amount of CdSe, the CdSe/TiO₂ photoanode exhibit three-dimensional structure, CdSe particle growing on planar structural CdSe/TiO₂. This structural CdSe/TiO₂ photoanode show the best photocatalytic performance owing to their good carrier transport pathway and high specific surface area. The stable photocurrent density reaches up to 5mA/cm², which is ten times than that of pure TiO₂ nanorods photoanode. Our investigations on the effect of structure of CdSe/TiO₂ to their photocatalytic performance provide meaningful references for designing efficient photoanode for water-splitting.

Wednesday, 21/Aug/2019 5:36pm - 5:48pm

Abstract ID: 324 / FBB-2: 9

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: DNA chips and nucleic acid sensors

Keywords: PCB microchip, Impedance measurement, dsDNA, PCR, Gold tagging.

An inexpensive and robust PCB platform for molecular diagnostics

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Growing advancements have immensely raised the requirement of devising low-cost fabrication strategies in biosensors. In this growth, the printed circuit board (PCB) technology has gained a lot of attention and is being immensely utilized for diagnostic purposes. This article represents usage of PCB based microchip for impedance measurement of the DNA products. Polymerase chain reaction (PCR) is used to obtain different concentration DNA products with DNA multiplied at 10, 20 and 30 cycles. The sensitivity of the detection is further enhanced by incorporating a gold nanoparticle tag to the DNA products through gold tagged primers which immensely enhance the functionality of the DNA products. The graphical abstract represents TEM image of the gold-conjugated DNA product (a) and Nyquist plot (b) as obtained through impedance measurement on PCB microchip corresponding to the three samples, namely DI water (—■—), 10 cycles non-tagged DNA product (—●—) and 10 cycle gold tagged DNA product (—◆—). A substantial reduction in impedance has been observed through the introduction of DNA in the DI water and further reduction is observed through gold tagging of the DNA products. A different signature has been obtained for tagged and non-tagged samples at lower frequencies which emphasis on the DNA functionality through gold tagging. Charge transfer resistance has reduced substantially from $\approx 25000 \Omega$ for non-tagged samples to $\approx 5000 \Omega$ for gold tagged samples (10 cycle PCR) signifying the importance of the presence of gold nanoparticles in the detection system. The interdigitated electrodes (electrode width $\approx 40 \mu\text{m}$ and interelectrode spacing $\approx 60 \mu\text{m}$) are fabricated on the PCB (having electroplated copper thickness $\approx 6 \mu\text{m}$) via photolithography and wet chemical etching route, which enormously reduces the fabrication cost. The impedance measurements are performed over the frequency range of 40 Hz -10 MHz with 250 mV excitation signal. Hence the reported microchip explains the importance of gold nanoparticle addition to the DNA samples for sensitivity enhancement on the robust and inexpensive PCB platform. The end goal of this strategy is to produce a detection chip to characterize the tagged/non-tagged PCR product through varied DEP capture frequency [1] and subsequent impedance measurement.

Thursday, 22/Aug/2019 9:24am - 9:36am

Abstract ID: 325 / FESC: 8

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: supercapacitors, wearable electronics, inkjet printing, Ni₂CO₃

Inkjet printing-assisted growth of Ni₂CO₃ nano-rods over fabric substrates for flexible and wearable supercapacitor applications

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Inkjet printing technology has recently attracted significant attention for manufacturing wearable and flexible electronic devices.[1] These devices can be easily mounted onto human skin for different applications such as; health monitoring devices, self-powered systems, electronic cloths, and other wearable displays. Wearable supercapacitors have lately reported to fulfill the energy requirement of the wearable electronics.[2] Here we report an inkjet-printed solid-state supercapacitor over the silk fabric substrates. All the inks were prepared using a water-based solution, and their rheological properties (surface tension, density, and viscosity) were carefully optimized to get the printable inks. Printing of graphene oxide (GO) and its reduction has converted the selective areas of the fabric as a conducting substrate. The NiCO compounds were digitally printed and hydrothermally grown over the conducting patterns of fabric substrates. The prepared nanostructures were characterized by FESEM, TEM, XRD and XPS which shows the excellent growth of Ni₂CO₃ nano-rod arrays over the fabric substrate. The open spaces between the nanorods are favorable for rapid charge transport and device stability. The assembled supercapacitor device with Ni₂CO₃ nanorods// AC exhibits excellent electrochemical performance upto 1.6 V in the LiClO₄ electrolyte. Figure 1 shows the schematic of the device assembly and FESEM image of the grown nanorods of Ni₂CO₃ over the fabric substrate. The prepared fabric based supercapacitor device delivers a high capacitance (~ 1400 F/g), long cycle life (> 5000 cycles), high energy and power density, and good rate capability. The fabric-based supercapacitor also shows excellent flexibility with negligible change in the device performance under different mechanical deformation conditions.

Wednesday, 21/Aug/2019 5:00pm - 5:12pm

Abstract ID: 326 / FBB-2: 6

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: 3D Scaffolds

Keywords: ECM, 3D in vitro modelling, neuroblastoma

Development of 3D engineered cell derived matrices by topological stimuli to assess how matrix anisotropy regulates tumoral cell proliferation and migration

Enrico Almici^{1,2}, Susanna Martín-Vañó^{3,4}, Joan Montero¹, David Caballero^{5,6}, Rosa Noguera^{3,4}, Josep Samitier^{1,2,3}

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Our focus is on engineered cell derived extracellular matrices (eCDM) development and exploitation. We believe that this approach could merge the capability of micro and nanobiofabrication techniques to tightly control topological and mechanical properties of 3D substrates, with natural structured scaffold production mimicking the extracellular matrix (ECM) of the target culture. We use a PDMS patterned substrate to study the topological influence on fibroblasts and neural Schwann cells in culture. After a decellularization procedure, we used the ECM produced to culture neuroblastoma tumoral cell lines and study its effect on their growth and invasiveness.

We employed PDMS replica moulding [1], to fabricate cell guiding templates displaying various geometric patterns. We first used the NIH3T3 fibroblasts cell line to produce ECM. At this point, the structure was decellularized resulting in a cell-free eCDM with specific features depending on the guiding template employed [2]. We characterized the ECM biochemical content by immunohistochemistry, its microfibers anisotropy by second harmonic generation and porosity variations by optical microscopy. In parallel, the Schwann immortalized cell line SW10 was also seeded on the eCDM and on the PDMS guiding template covered with gelatin. Our main interest is to study how Schwann cells behave in response to the ECM produced and determine which modifications arise in the final decellularized scaffold. Our final goal is to use the eCDM produced to analyse in vitro and ex vivo, from primary samples, neuroblastic tumoral cells proliferation and migration dynamics [3].

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Abstract ID: 327

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Carbon Nanomaterials

Keywords: Graphene, hexagonal boron nitride, hybrids, magnetism

Switchable ferro-magnetism and more in layers of 2p block elements

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Atomically thin layers made of elements in the 2p block of the periodic table – graphene, hexagonal boron nitride (hBN) and their solid-solutions or hybrids, are not only the lightest but also mechanically one of the most stable and resilient layered self-assemblies ever found. They continue to intrigue us in terms of their rich physics and the consequent promise of technological applications, notwithstanding the simplicity of their valence configurations – described entirely by s and p electrons, particularly the latter, when it comes to low energy properties within few eVs where most of our optical and electronic devices work. These layers derive their uniquely tunable electronic and magnetic properties from their three coordinated bipartite structure, which facilitate the interplay of two basic properties of electrons -- their delocalization meant to reduce their kinetic energy, and localization of electrons of opposite spins in the two sub-lattices in order to reduce Coulomb repulsion among them. Physical and chemical functionalization tilts the balance between the two and leads to a plethora of non-trivial ground states. In this talk, based on first principles calculations and mean-field Hubbard model, we will discuss primarily how graphene and graphene-hBN hybrids can be turned into ferromagnetic metal, semiconductor and a half-metal possibly at room temperature, by tuning the interplay of kinetic energy and Coulomb repulsion through localization of electrons induced reversibly by application of electric field, or irreversibly due to specific graphene-hBN hybrid structures. As an example of reversible functionalization, we will specifically discuss how electron localization due to inhomogeneously applied electric field can lead to nearest neighbour ferro-magnetic ordering in graphene sheets and ribbons as a general property of bipartite lattices. We will also discuss how magnetic ordering between graphene islands embedded in hBN can be designed to retain non-zero magnetic moments at room temperature.

Wednesday, 21/Aug/2019 6:27pm - 6:39pm

Abstract ID: 328 / FC: 13

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalysis for pollution control

Keywords: Photocatalysis, Vanadium pentoxide, Wastewater decolourization

Hemin (Fe+3-porphyrin) anchored V2O5 nanowires for solar light based photocatalytic decolourization of MB dye and Industrial wastewater

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Transition metal oxide based semiconducting materials are widely used photo-catalysts in UV and visible range of solar spectrum. Vanadium pentoxide (V2O5) is a transition metal oxide and works as an effective functional material for photo-degradation of complex dyes present in water solution. On solar light irradiation, the electrons (e^-) at the valence band of V2O5 gets excited and jump to the conduction band and leave holes (h^+) behind at the valence band. These electrons and holes react with water molecules and form hydroxyl radical (OH^\bullet), which is a highly reactive oxidizing agent and degrades complex dye molecules. Although, V2O5 is a fine photo-catalyst but it has some drawbacks which decreases its performance. The major issues are electron/hole recombination losses and absorption of small part of available solar light spectrum at the surface of V2O5 nanostructures. Hemin (Fe+3-porphyrin) is an iron containing compound which shows excellent solar light trapping property. Hemin, anchored with V2O5 serves dual function by providing a conducting path for electrons present at the conduction band of V2O5 to avoid recombination losses and absorbing the larger portion of solar light spectrum to improve the photocatalytic performance. In this study we utilized Hemin anchored V2O5 nanowires (H-V2O5) for photocatalytic decolourization of methylene blue (MB) and an industrial wastewater dye under solar light irradiation. Approximately 25% faster decolourization rate was achieved in case of H-V2O5 in comparison with pure V2O5 for MB dye. H-V2O5 is also tested as a photo-catalyst for decolourization of a complex industrial wastewater dye (Obtained from Common effluent treatment plant (CETP), Jodhpur, India). The graphical abstract shows synthesized V2O5 nanowires and UV-Vis absorbance spectra of the MB dye at regular interval of time. The detailed characterization of the synthesized materials was conducted and significant information about material properties were studied. This study suggests H-V2O5 as an efficient photo-catalyst for MB and wastewater dye decolourization utilizing the solar light as a source of energy.

Abstract ID: 329**Symposium 1: Functional Biomaterials and Biosensors (FBB)****Poster Presentation**

Topics: Applications in orthopedic, cardiovascular, dental, nerve tissues, etc

Keywords: surface morphology, SEM, AFM, antibacterial activity

Solubility, morphological and antibacterial properties of biomaterials with graphene

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The dental biomaterials are made out of biocompatible materials like hydroxyapatite, bioglasses, bioceramics and also, as of recently, nanopowders with graphene. We have previously reported, in our past papers, that the performance of biomaterials has been improved by the incorporation of graphene and the improvement was especially enhanced when the graphene was used in the dental materials [1, 2]. In this study, we want to report some results on the solubility, morphological and antibacterial tests of the biomaterials with the graphene oxide with SiO₂, and ZrO₂ respectively. Five experimental biomaterials were made using the BisGMA organic matrix (synthesized in our laboratory)/TEGDMA(Aldrich) and inorganic phase: (HA-SiO₂, barium glass, GO-SiO₂: 1%, 0,8% - for GS1, GS2: and HA-Zr, barium glass, GO-ZrO₂:1%, 0,8% for GZ1, GZ2) and GC (HA-Zr, HA-SiO₂, colloidal silica; barium glass) composite without graphene, in 20/80 proportions of weight. The solubility test, according to ISO 4049/2000 on the used specimens (15x1mm) which were photochemical initiated with visible light cured (Woodpeker LED Lamp) in water and artificial saliva were measured at 1, 7 and 30 days. The surface and structure of the biomaterials, in the initial state and after 30 days of storage in saliva and water, were analyzed by AFM (NTEGRA Spectra (NT-MDT)) in order to observe surface roughness (Ra) and SEM (Inspect F-FEI) in order to observe the biomaterials surface effects. The antimicrobial activity materials were evaluated using the agar diffusion method. The bacterial strains were taken from Escherichia coli ATCC 25922 (Gram negative) and Staphylococcus aureus ATCC 25923 (Gram positive). We used the paper disc method and the wells method to gather readings at every 24h and 48h. The interaction mechanism between polymer/graphene/bioglasses/nanofillers used in dental biomaterials, depends on: polarity, molecular weight, hydrophobicity, particles size and shape, reactive groups, etc., present in their composition. The results suggest that the difference in surface roughness between the composites could be related to their composition, the conversion degree and the immersion time of the specimens. For the water immersed samples, there were large differences between the measurements taken at 7 and 30 days, respectively. After the accelerated artificial aging a homogeneous structure can be observed, presenting gaps when the nanocomposite was stored in distilled water. Artificial saliva didn't attack the surface of the composite, instead, it was maintained homogeneous. Experimental biomaterials with a higher graphene percent presented significantly higher water sorption values after water immersion (p < 0.001). The bacterial inhibition assay revealed an antibacterial activity for all the samples, but the best activity is against S. aureus bacteria for composites with GO-SiO₂ graphene

Abstract ID: 330**Symposium 3: Functional Catalysis (FC)****Poster Presentation**

Topics: Catalysis for pollution control

Keywords: Nanofibers, Photocatalytic properties, Solution blow spinning

Photocatalytic efficiency of PVDF/TiO₂ nanofibers produce by SBS process

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In the development of nanomaterials, polymeric nanofibers are in expansion in different knowledge areas. They can be processed by a number of techniques such as Template Synthesis, Self-Assembly, and Electrospinning. Among various chemical or physical synthetic approaches, electrospinning appears to be the most straightforward and versatile technique for generating 1D nanostructures, however, this technique uses a high voltage electrical field to induce the formation of nanofibers. The use of high voltage is a concern due to the potential combination of sparks and flammable solvents. Recently an alternative method named solution blow spinning (SBS) was developed to produce nanofibers¹. In this process, without the use high voltage, the polymeric solution is elongated by the force of a high-speed gas stream and as the solvent evaporates, during the spinning process, the elongated fiber becomes solid. The technique allows the fabrication of continuous fibers with diameters down to a few nanometers and with complex architectures, such as core-shell fibers or hollow fibers, also enables to produce structures ranging from single fibers to ordered arrangements of fibers. Polyvinylidene fluoride (PVDF) is one type of polymer that can be used to produce nanofibers². PVDF is a semi-crystalline polymer which has good mechanical properties, good chemical resistance, and excellent processability. In addition, blending with inorganic materials, especially nanoparticles such as TiO₂, has attracted great attention due to the possibility of promoting photocatalytic properties in water purifying membranes³. Despite the potential, the fabrication of PVDF/TiO₂ nanofibers allows their easy separation after a photochemical reaction and reuse, which increase their practical application. In this work was investigated the structure, morphology and photocatalytic efficiency of PVDF/TiO₂ nanofibers produce by SBS process. The results showed the formation of homogeneous, straight, smooth, and randomly dispersed nanofibers with photocatalytic properties.

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Thursday, 22/Aug/2019 9:36am - 9:48am

Abstract ID: 331 / FLNM: 9

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nanomechanics

Keywords: Graphene sheets, Multiscale modelling, Finite element method, Dihedral energy, Nanomechanics

Modified Multiscale Computational Framework for the Nonlinear Dynamics Response of the Two-Dimensional Nanomaterials

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A modified multiscale computational framework based on finite element method is employed to investigate the nonlinear dynamic characteristics of two-dimensional nanomaterials. The present model is refined for the accurate prediction of bending modulus including dihedral energy term in the constitutive law and constitutive law is established in the framework of second-generation reaction empirical bond order potential. The deformations at atomistic and continuum level are coupled through the Cauchy- Born rule. For the numerical demonstration, present formulation is employed to study the nonlinear dynamic response of carbon nanotubes and graphene sheets incorporating material and geometric nonlinearities and their effects on the nonlinear dynamic response are quantified.

Abstract ID: 332

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Composite structural materials

Keywords: PCPs/MOFs, Superhydrophobicity, Oils spill cleanups, Composite materials

Temperature Stable Novel Porous Coordination Polymer (PCP) based artificial Lotus Leafs for Applications in Energy and Environment

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Porous coordination polymers (PCPs), or metal-organic frameworks (MOFs) are emerged as potential materials of the decade, particularly for gas storage, separation, catalysts, and sensors etc. However, PCPs existing in the literature were mostly instability with respect to moisture and bulk water. Beyond these traditional PCPs, we achieved first time four new superhydrophobic porous coordination polymers (SPCPs), with molecular formulas, $Zn_4(u^3-OH)_2(BTMB)_2 \cdot Guest$ and $Zn_2M_2(u^3-OH)_2(BTMB)_2 \cdot Guest$ ($M = Co$ and Ni) (SFPCP-1-Guest; $BTMB^{3-} = 1,3,5$ -benzenetris(m-benzoate)) and $Pb(H-BTMB)(DMF) \cdot (1)$. The obtained first series three new PCPs containing $[Zn_4O]^{6+}$ $[Zn_2M_2O]^{6+}$ ($M = Co$ or Ni) bimetallic cluster core with open metal sites (OMSs) exhibited distinct isosteric heats of adsorption and surface areas due to the difference in their open metal Lewis acidic sites of solvent-free state. These interesting PCPs, possesses an aromatic terminating surface that is highly corrugated over the nano-scale. Additionally, these PCPs exhibit remarkable superhydrophobic properties with contact angles of, 155.5° 159.3° and 160.8° respectively for Zn-Zn, Zn-Co and Zn-Ni analogues. In this presentation, we discuss, synthesis, structures, characterizations, properties, and applications these novel PCPs. Remarkably, SPCP-1 unveiled superhydrophobic self-cleaning behaviour due to the formation of Hierarchical structures. Furthermore, the properties of superhydrophobicity make this PCP adsorb organic solvent from water surface without decomposition following submerging in water. We also discuss the gas storage and separation properties of these new PCPs. This study can provide a roadmap to design and synthesis of novel porous materials for the applications in energy and securing the environment.

Key Words: PCPs/MOFs, Superhydrophobicity, Oils spill cleanups, Composite materials.

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Abstract ID: 333

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalytic Materials & Mechanisms

Keywords: hydrogen generation, minerals, heterogeneous catalysis, recyclability, ammonia borane

Self-healing Catalysis for the Hydrolytic Dehydrogenation of Ammonia Borane

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Sustainable catalysts based on earth-abundant elements are considered as economical alternatives to precious-metal-bearing catalysts and could be impactful for many applications. Self-healing sustainable catalysts, which in addition to their ‘green’ characteristic can spontaneously repair themselves without the need of applying heat, pressure or electrochemical bias, are particularly desirable for numerous large-scale chemical processes. Herein, we present the discovery of such a catalyst, named SION-X, for the hydrolytic dehydrogenation of ammonia borane (AB, NH_3BH_3). SION-X is the synthetic form of a mineral and, following in situ reduction, catalyzes the release of almost all 3 equivalents of hydrogen (H_2) from 1 equivalent of AB. During the reaction, the metal ions in SION-X are reduced to metallic nanoparticles, and after the reaction, following exposure to air, they are oxidized re-forming SION-X. As a consequence, the catalytic activity of SION-X toward the production of H_2 from AB remains unchanged over many cycles. The self-healing catalysis of SION-X in the absence of any extra energy input gives a new perspective in heterogeneous catalysis for energy-related applications.

Thursday, 22/Aug/2019 12:24pm - 12:36pm

Abstract ID: 334 / FTF: 8

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Nanostructured and Architecturally Designed Coatings, Smart Surfaces

Keywords: Nanocellulose, Ultrathin films, Water Interactions

Specific Water/Vapor Uptake of Ultrathin Films of Cellulose: Paving the Way for New Responsive Materials from Renewable Polymers

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Cellulose is the main structural component of all plant fibers. Recent technology has enabled the top-down isolation of the nanosized supramolecular units from within the fiber and the possibilities of these nanocellulosic building blocks in applications of materials science were recently reviewed.¹ In this presentation, we focus on the specific applications of nanocellulose in ultrathin films whose interactions with water and water vapor were scrutinized. Contrary to the common assertions, nanocellulose is not exclusively hydrophilic but in fact, amphiphilic (although it is highly hygroscopic) and this amphiphilicity leads to a distinct, controllable behavior with water, elaborated here from the physico-chemical perspective. Generally, the high water uptake of nanocellulose is viewed as a nuisance, resulting in, e.g., strength reduction of its composite materials. By contrast, we want to see the specific nature of its water interactions as an asset with nanocellulose.

Several aspects of this work have already been published²⁻⁴ whereas fresh data will also be presented, linking the data to general considerations on diffusion, porosity, and crystalline/amorphous characteristics of the cellulose in use. The results demonstrate the potential of ultrathin nanocellulose films in applications such as sensors and actuators. Overall, we advocate the vision where the specific properties of renewable polymers would be given more attention instead of the approach where renewability and sustainability are their sole assets in materials science.

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Thursday, 22/Aug/2019 10:12am - 10:24am

Abstract ID: 335 / FLNM: 12

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Chemistry of 2D Materials for Energy, Catalysis and Sensing Applications

Keywords: Noble metal nanoplates, MOF nanosheets, Hybrid nanomaterials, Solution-phase growth, Organic peroxides detection

Solution-Phase Synthesis of Noble Metal (Ag, Au, Pd) Nano-plates Decorat-ed 2D Metal-Organic Frame-work Hybrid Nanomaterials

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Two dimensional (2D) layered nanomaterials such as graphene oxide (GO), transition metal dichalcogenides (TMDs) and boron nitride (BN) have attracted increasing research interest, due to their unique physical and chemical properties. Very recently, 2D metal-organic framework (MOF) nanosheets, as a new member of the 2D family, were successfully prepared. As known, MOF is a crystalline porous material constructed by coordination of metal ions or clusters with polytopic organic ligands, possessing many promising features, such as tunable structure and function, large surface area, and highly ordered pores. In our previous work, a serial of 2D MOF nanosheets with thickness less than 10 nm were synthesized using the surfactant-assisted method. Interestingly, the 2D MOF nanosheets show peroxidase-like activity. Recently, several hybrid composites showing enhanced catalytic activity due to the synergistic effect have been reported. Inspired by that, we demonstrated 2D MOF nanosheets (Cu-TCPP and Cu-TCPP(Fe)) can be used as the template to growth of silver (Ag), platinum (Pd) and gold (Au) nanosheets at ambient conditions. Importantly, The noble metal plates on the surface of 2D MOF are uniform and possess ultrathin structure, which are the ideal materials for catalysis due to accessible active sites, fast electron transfer, high stability, and good solution-dispersion. The integration of noble metal plates with 2D MOF nanosheets displays synergistic properties and functions. As a proof of the power of such materials, the obtained Pd/Cu-TCPP(Fe) hybrid nanomaterials show peroxidase-like activity, which exhibits enhanced activity compared to Pd nanoplates, Cu-TCPP(Fe) nanosheets, and the mixture of both. On the basis of their high catalytic activity, a simple, fast and highly sensitive fluorescence method was developed to detect trace amounts of explosive residues (organic peroxides) in environment.

Thursday, 22/Aug/2019 12:00pm - 12:12pm

Abstract ID: 336 / FCM-3: 6

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Smart Composites

Keywords: Carbon Nanotubes, Composite, Friction

A novel Carbon Nanotubes based grease formulation and its unique lubricating performance

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The remarkably beneficial frictional behavior of carbon nanotubes was observed in numerous research projects conducted in the last two decades, these include nano-scale experiments using AFM and similar techniques as well as a wide range of tribometer tests. The results produced in these studies were confirmed again in our experiments where the beneficial friction-wear impact of carbon nanotubes added to the lubricating oil was clearly observed in full-engine tests [1]. Unfortunately some shortcomings still remain to be solved in order to consider industrial application of this solution, the most problematic one of them being the reagglomeration of the cnts dispersed in engine oil.

One smart solution definitely avoiding the cnt reagglomeration problem is a formulation of a cnt-oil composite where a minimum level of 1% cnt mass content was exceeded making the product have a consistency similar to grease. The experiments described in this paper prove that delivering a high ultrasonic or shear stress energy converts a fluid pre-mixed cnt-oil dispersion in grease in the span of a few seconds. The product is a composite where we observed cnt scaffold similar in form and primary function to the standard network obtained through lithium or calcium soap in commercially used greases.

In addition to their primary networking function carbon nanotubes can significantly modify the friction process, eventually providing unique lubricating properties to the grease they form. Using Raman spectroscopy we documented that the cnt delivered to the friction components with grease were permanently incorporated into the polymer surface tested in Amsler tribometer, where they reduced friction and wear significantly. The same effect was observed after a long-running test performed for a standard metal ball bearing. For some application a hybrid grease structure based on standard soap network enhanced through cnt addition can be most effective. We tested such a hybrid product revealing a promising cnt dispersion improvement during the ball and roller bearing run, eventually obtaining a stable, non-degrading cnt structure. The processes and phenomena described above have been documented with: Raman spectroscopy, EDS mapping, 3D topography, confocal and ESEM microscopy.

The proposed high energy – short duration ultrasonic-based method for the novel grease formulation can easily be adopted in the large scale production replacing conventional process based on slow chemical reactions performed in a high temperature and pressure environment.

Research presented was performed within the statutory work, project no. 05/52/PNCN1838.

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Abstract ID: 337

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Photocatalysis

Keywords: Titanium dioxide, Hydrothermal treatment, Photocatalytic activity, Methylene blue degradation, Metal-doped

Characterization of Metal-doped Titania nanobeads photocatalyst synthesized by hydrothermal method

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Titanium dioxide (TiO₂) is one of the well-known ceramic materials and widely used in many research fields because of its low cost, high oxidation-reduction performance and high photocatalytic activity. A defect of TiO₂ is the wide band gap (~3.2 eV), limiting its charge separation. In this study, we synthesized metal-doped TiO₂ nanobeads by hydrothermal treatment to enhance the photocatalytic effect of TiO₂. In autoclave, as the temperature increases at a limited volume, the pressure of the solution increases and then the reactivity of the molecules increases. We could prepare TiO₂ nanobeads by hydrothermal treatment at low temperature due to previous principle. Octadecylamine (ODA) had hydrophobic long-chain alkyl group and hydrophilic amino group. In the solution, hydrophobic groups tended to self-organize into micelles structure. Titanium tetraisopropoxide (TTIP) participated in hydrogen-bonding interactions with amino groups of ODA to form inorganic-organic composites. The kinds of metal doping were iron, vanadium and nickel. The XRD, SEM and TEM characterized the crystallinity and morphology of the metal-doped TiO₂ nanobeads. We could confirm the surface area, pore volume and pore size of TiO₂ nanobeads by BET analysis. We compared with the photocatalytic activity of the metal-doped TiO₂ nanobeads and non-doped TiO₂ nanobeads. The photocatalytic effect was measured by the degree of methylene blue degradation. The metal-doped titania beads had higher photocatalytic effect than the standard TiO₂ bead because the electrons were easily excited by the metal. For this reason, the photocatalytic activity of TiO₂ beads could be enhanced which make it appropriate for a variety of applications ranging from photocatalyst, energy storage and conversion, Li-ion batteries.

Abstract ID: 338 / Poster: 43

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Applications in orthopedic, cardiovascular, dental, nerve tissues, etc

Keywords: nano-capsules, surface morphology, SEM, AFM, cytotoxicity

Influence of various whitening agents upon biomaterials used in dentistry

Ionela - Amalia Mazilu¹, Marioara Moldovan², George Popescu³, Andrei Moldovan⁴, Codruta Sarosi², Violeta Popescu¹

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The idea of incorporating nanoparticles into the gel matrix to develop a natural product with remineralization and whitening capabilities has been recently explored by lots different researchers that consider the use of natural whitening gels containing nano-capsules being considered innovative. These experimental natural whitening gels are highly susceptible to remineralizing the partially demineralized enamel through calcium and phosphate phases deposits on top of the remaining apatite crystallites. The objective of this paper was to study the influence of various whitening agents (experimental natural bleaching gel G24® [nano-capsules (nanohydroxyapatite, extract natural, PLC)] and commercial BrightBleach®, upon the surface morphology and color of various restorative biomaterials [Nanofill®, AT&M Biomaterials Co., Ltd. and 3 experimental biomaterials (P11, P31, P61) which were light-cured initiated (Woodpecker LED Lamp)], along with the cytotoxicity test. Each of the biomaterials were prepared in Teflon molds (1 × 1,5 mm), and further divided into three groups [n = 5 controls were placed in artificial saliva and the other two groups of n = 5 were placed in coffee, for 10 and 30 days and bleached with experimental and commercial gels]. Color measurements were taken before and after the immersion in solutions and after bleaching, using a UV-Vis spectrophotometer (JASCO). These were than compared to digital images, using the original software application "Discolor". Two methods were used: Atomic Force Microscopy (AFM - NTEGRA Spectra (NT-MDT)), to observe surface roughness (Ra) and Scanning Electron Microscopy (SEM – Inspect F-FEI), to observe the effects on biomaterials surface morphology. For cytotoxicity testing, we used both cell lines: human dermal fibroblasts (HDFa) and the dental follicle stem cells. The samples were incubated with culture medium at 37°C, the proportion of 1 ml average /3 cm² surface composite sample for 24 and 72 hours, before and after the whitening process. The two-way ANOVA test was used to evaluate the results. All biomaterial samples immersed in coffee showed significant coloration compared to baseline values (P<0.05). Discoloration in samples immersed in artificial saliva was not significant compared to baseline (P>0.05). The interaction between immersion time and bleaching gel type was also significant (p<0.002). ΔE values obtained from the UV-Vis spectra and digital imagine were significantly different to all four types of biomaterials stored in coffee (P<0.05); whilst no significant difference was observed in the ones stored in artificial saliva (P>0.05). Also no major changes of the dental composites' surface morphology were observed. The most important effect of the decrease in viability was recorded for samples P11 and Nanofill®, on fibroblasts. This effect was greatly reduced dental follicle stem cells and visible only for P11.

Thursday, 22/Aug/2019 12:00pm - 12:12pm

Abstract ID: 339 / FTF: 6

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Optical, electrical and magnetic properties of thin films

Keywords: Scintillation materials, Raman spectroscopy, Perovskites

Raman spectroscopy of doped single crystalline films of perovskites grown using liquid-phase epitaxy method

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Scintillators are special group of materials able to convert high-energy X-rays or γ -rays into photons in UV-visible range. Historically, CaWO₄ and ZnS-based powders were recognized as potential scintillators for X-ray detection in the late XIX century. In the late 1940's single crystals of NaI:Tl and CsI:Tl were used as scintillators, and then oxide-based CdWO₄ and Bi₄Ge₃O₁₂ scintillators for versatile applications in the field of high-energy physics were popularized [1].

Ce³⁺ doped single crystals (SC) of perovskites e.g. YAlO₃ (YAP) and LuAlO₃ (LuAP) have become prevalent for use as scintillators since the 1980's. During the last decade single crystalline films (SCFs) of Ce³⁺ doped YAlO₃ [2] and LuAlO₃ [3], as well as the Ce³⁺ and Mn²⁺ doped TbAlO₃ (TbAP) perovskites [4] were synthesized using liquid-phase epitaxy method onto YAP substrates.

In this paper we present for the first time Raman spectroscopy investigations of undoped YAP, Mn²⁺ doped TbAP and Ce³⁺ doped YAP and LuAP single crystalline films (SCFs) grown onto YAP substrates. In order to record undisturbed Raman spectra of SCF and YAP substrate the samples were broken and the spectra of particular parts of the cross-section were measured. The evolution of Raman spectra and Raman maps recorded for YAP:Ce@YAP, TbAP:Mn@YAP and LuAP:Ce@YAP epitaxial structures allow a distinction between SCF and the substrate and furthermore allow identification of a transition layer between SCF and the YAP substrate. The transition layer can be treated as solid solution of the SCF and YAP substrate compositions, with gradually changing occupancy of twelve coordinated sites of Y³⁺ ions by Tb³⁺ or Lu³⁺ ions.

Acknowledgments. This work was supported partially by the Research Projects of the Polish Ministry of Science and Higher Education 06/65/DSPB/5182.

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Abstract ID: 340

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nanomechanics

Keywords: Fracture toughness, graphene oxide, molecular dynamics

Nanomechanics of Graphene Oxide Nanosheets

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Two dimensional materials possess fascinating electronic, optical and physical properties, however, one major drawback limiting their large-scale application is susceptibility to fail in a brittle fashion when loaded. Considering graphene as an example, we demonstrate that such a limitation can be alleviated by suitably functionalizing the basal plane of carbon atoms with oxygen and hydrogen atoms, a material commonly known as graphene oxide (GO). A nonlinear finite element fracture analysis coupled with in-situ transmission electron microscopy based tensile testing was implemented to quantify the nonlinear fracture toughness of multilayered GO. Our calculations predict a fracture toughness of 39 J/m² for GO as compared to a JIC of 16 J/m² of bare graphene¹, a nearly 250% improvement. Experimental observations coupled with molecular dynamics simulations revealed a transition in the failure behavior from interplanar fracture, common for bulk GO, to intraplanar fracture, which dominates failure in monolayer GO. Additionally, MD simulations indicated that the elastic release from the propagation of intraplanar cracks initiates global fracture due to interlayer load transmission through hydrogen bond networks within the gallery space of the GO nanosheets. For multilayer samples with an elliptical crack, a crack arresting mechanism was identified as the main contributing factor for the higher fracture toughness as compared to graphene. Our simulations indicated that the interactions among functionalized atoms in constituent layers and distinct fracture pathways in individual layers, due to a random distribution of functionalized carbon atoms in multilayers, restricted the growth of a preexisting crack. The results inspire potential strategies for overcoming the relatively low fracture toughness of 2D materials through chemical functionalization.

Abstract ID: 341

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Additive manufacturing Applications

Keywords: gypsum-based composites, robocasting, setting, rheology, microstructure

The setting and rheological behavior of gypsum-based composites used for 3D robocasting

Chuanbei Liu^{1,2}, Jianming Gao^{1,2}, Yasong Zhao^{1,2}, Xuemei Chen^{1,2}

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3D robocasting is a promising method to improve the mechanical strengths of printed gypsum products. In this study, the gypsum-based composites (GC) mainly comprising α -hemihydrate gypsum, polycarboxylate, hydroxypropyl methyl cellulose, starch ether and ultra-dispersed attapulgite were prepared and used for 3D robocasting. The setting time and rheological properties of the GC slurry were measured by vicat apparatus and rotational rheometer, respectively. Besides, the early hydration and microstructure of the GC slurry were studied by environment scanning electron microscope coupled with liquid nitrogen cooling. It has been proven that the setting time and rheological properties of the CC slurry are key performance parameters determining whether it can be used for 3D robocasting and closely related to the early hydration and microstructure. The above-mentioned admixtures would promote the flocculating or deflocculating between hemihydrate particles and therefore modify the rheological properties. Besides, these admixtures would also absorb on the surface of hemihydrate particles and therefore prolong the setting time. As a result, the GC slurry has much higher yield stress, final viscosity as well as longer setting time than the pure gypsum plaster (G) paste. Besides, the GC slurry changes from solid like to liquid like behavior at cross-over shear stress and exhibits rapid recovery of shear modulus after stress removal. These properties above proves to be beneficial to the 3D robocasting of the GC slurry.

Abstract ID: 342

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Synthesis, Controllable Growth and Characterizations

Keywords: Solvent-less, Solid state grinding route, Bimetallic, Chalcogenides, Nanocrystal.

A Solvent-less Solid State Grinding Method for the Synthesis of Dispersible Semiconducting Bimetallic Sulfide (Ternary) Nanocrystals

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A Solvent-less Solid State Grinding Method for the Synthesis of Dispersible Semiconducting Bimetallic Sulfide (Ternary) Nanocrystals

Abhijit Bera and Bhagavatula L. V. Prasad*

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A rational synthetic method that produces monodisperse and air stable metal sulphide colloidal quantum dots (CQDs) in organic nonpolar solvents (hot injection method) using octyl ammonium octyl dithiocarbamate (C8DTCA) as a sulfur source, was developed. The high reactivity of C8DTCA, in presence of primary amines, towards metal complexes is exploited to achieve this purpose. This novel technique is generic and can be applied to prepare diverse CQDs, like CdS, MnS, ZnS, SnS, In₂S₃, including more useful and in demand PbS CQDs and plasmonic nanocrystals of Cu₂S. Based on several control reactions, it is postulated that the reaction involves the in situ formation of a metal-C8DTCA complex which then reacts in situ with oleylamine at slightly elevated temperature, decomposes to metal sulfide CQDs at a controlled rate leading to the formation of large scale of monodisperse CQDs. Tunable and desired crystal size could be achieved by controlling the precursor reactivity by changing the reaction temperature and reagent ratios. Finally the photovoltaic devices fabricated from PbS CQDs displayed a power conversion efficiency of ~5 % that is comparable with the reported values of devices prepared with PbS CQDs obtained by the standard methods.

Interestingly, all of these individual metal sulfide materials are also synthesized using an atom-economy and solvent-less green approach, by simple and convenient solid state grinding route. This simple methodology could be used to prepare <3 nm nanocrystals like Ag₂S, PbS and Cu₂S which are otherwise difficult to prepare by the conventional and high temperature solution routes. Not only the individual metal chalcogenides, but also some important bimetallic chalcogenides (S or Se) like AgBiS₂, AgInS₂, and CuInS₂ etc are also demonstrated to be synthesized using an atom-economy and solvent-less green approach, by simple and convenient solid state grinding route. Interestingly, some of these bimetallic chalcogenides like AgBiS₂ and CuInS₂ shows comparatively good photovoltaic response. The results will be presented in the poster.

Key Words: Solvent-less, Solid state grinding route, Bimetallic, Chalcogenides, Nanocrystal.

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3. A. Bera and Bhagavatula L. V. Prasad, A Solvent-less Solid State Grinding Method for the Synthesis of Dispersible Semiconducting Bimetallic Sulfide (Ternary) Nanocrystals (To be communicated)

Wednesday, 21/Aug/2019 4:24pm - 4:36pm

Abstract ID: 343 / FCM: 3

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Polymeric composites

Keywords: Responsive fabric, Micro-climate, Body heat, Metabolism.

Nanocomposite membrane for human thermoregulation

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Human body release heat in four ways conduction, convection, evaporation and radiation. The normal core temperature of a human body is around 37°C, enzymes and proteins may destroy, and metabolism may dis-function if the core temperature is above 45°C or below 34°C, and lead to death. To overcome such limitations, we develop an Evaporative-Radiative-Convective Fabric (ERCF) that control the personal microclimate of the human body by body cooling (evaporation of perspiration, air convection and emission of radiation of human body directly to the environment). In this work, we fabricate the thermo-moisture sensitive nanocomposite membrane which is super evaporative, radiative and can facilitate the convection process of the human body. We processed the sensitive membrane to fabricate a textile which can warm up the human body by releasing body heat. The material we develop has robust mechanical property for the longevity of the material, high water vapor and air permeable. The fabricated materials can control the microclimate of the human body by auto actuate the wearables, and the switching temperature of the material is around 37°C which is the ideal temperature for human body if the body temperature is high the material will be more open in order to facilitate the releasing body heat. Microclimate controlled fabric can release approximate 85% of body heat.

Abstract ID: 344

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Solar Cells

Keywords: Solvent-less, Solid state grinding route, Bimetallic, Chalcogenides, Nanocrystal.

**A Solvent-less Solid State Grinding Method for the Synthesis of Dispersible
Semiconducting Bimetallic Sulfide (Ternary) Nanocrystals**

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A Solvent-less Solid State Grinding Method for the Synthesis of Dispersible Semiconducting
Bimetallic Sulfide (Ternary) Nanocrystals

Abhijit Bera and Bhagavatula L. V. Prasad*

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A rational synthetic method that produces monodisperse and air stable metal sulphide colloidal quantum dots (CQDs) in organic nonpolar solvents (hot injection method) using octyl ammonium octyl dithiocarbamate (C8DTCA) as a sulfur source, was developed. The high reactivity of C8DTCA, in presence of primary amines, towards metal complexes is exploited to achieve this purpose. This novel technique is generic and can be applied to prepare diverse CQDs, like CdS, MnS, ZnS, SnS, In₂S₃, including more useful and in demand PbS CQDs and plasmonic nanocrystals of Cu₂S. Based on several control reactions, it is postulated that the reaction involves the in situ formation of a metal-C8DTCA complex which then reacts in situ with oleylamine at slightly elevated temperature, decomposes to metal sulfide CQDs at a controlled rate leading to the formation of large scale of monodisperse CQDs. Tunable and desired crystal size could be achieved by controlling the precursor reactivity by changing the reaction temperature and reagent ratios. Finally the photovoltaic devices fabricated from PbS CQDs displayed a power conversion efficiency of ~5 % that is comparable with the reported values of devices prepared with PbS CQDs obtained by the standard methods.

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Key Words: Solvent-less, Solid state grinding route, Bimetallic, Chalcogenides, Nanocrystal.

References

1. A. Bera, D. Mandal, P. N. Goswami, A. K. Rath and Bhagavatula L. V. Prasad, *Langmuir*, 2018, 34, 5788–5797.

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3. A. Bera and Bhagavatula L. V. Prasad, A Solvent-less Solid State Grinding Method for the Synthesis of Dispersible Semiconducting Bimetallic Sulfide (Ternary) Nanocrystals (To be communicated)

Abstract ID: 345

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalysis for pollution control

Keywords: XRD; NEXAFS; Raman Spectra; Photocatalyst, MB.

The contribution of surface defects on the local atomic structure and photocatalyst properties of Fe: CeO₂ NPs

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The Ce³⁺ ions in the vicinity of oxygen vacancy (Ov) at the surfaces of cerium dioxide nanoparticles (CeO₂ NPs) are active sites and contribute significantly on the photo-catalyst activity. In this work, the structural and photo catalyst applications of Ce_{1-x}Fe_xO_{2-δ} (x) NPs synthesized through simple co-precipitation technique have been investigated. X-ray diffraction (XRD) patterns revealed that all the samples possess single phase fluorite structure without any foreign peak. The crystallite sizes decreased progressively as the Fe content increase and ranging between 8.9 and 6.5 nm. The decrease in the crystal domains, further illustrated by TEM micrographs images, is related to decrease the crystal quality and increase the oxygen deficiency over the surfaces of nanostructured Fe: CeO_{2-δ} (δ = Ov Ce³⁺). The Ov has been traced via Raman spectra, from which the F_{2g} Raman phonon mode at 462 cm⁻¹ showed a broadening and red shift tendency to lower frequency in sequence with further iron content, indicating to that the Fe dopant induces further oxygen vacancies. The NEXAFS spectral feature at Fe L_{3,2} edges signified that the Fe ions occupied partial sites of Ce ions in the CeO₂ matrix with mixed valence state of Fe³⁺ and Fe²⁺. Hence, the photo-catalyst activity of the samples was implemented on the methylene blue (MB) dye decomposition under the sunlight light. The catalyst efficiency and dissociation of adsorbed water molecules at the surfaces of NPs enhanced as the Fe doping content increase that related to Fe²⁺/Fe³⁺ redox cycles and creation of Ce³⁺/Fe²⁺ profound bands induced via Ov, which causes a suppression of the recombination of photo-generated electron–hole pairs.

Abstract ID: 346

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Nanocomposites

Keywords: dye release, rice husk silica, rice husk, polycaprolactone, PCL, biodegradation polymer, nanofiber

Release control on the specific surface area of rice husk silica immobilized in polycaprolactone nanosheet by electrospinning.

Sinae Song¹, Guijun Choi², Moongyu Kim², Heetaik Kim^{1,2}

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Releasing control from rice husk silica nanoparticle(NP/SiO₂) with diverse specific surface area immobilized in polycaprolactone (PCL) nanofiber sheet was conducted depending on the diverse nanoporosity of NP/SiO₂ by decomposing of PCL. The nanoporous silica was extracted from rice husk as known biomass and synthesized with controlling of the factors such as pH, amount of used rice husk ash and aging time, drawing the specific surface area and pore size 240.09 ~ 740.77 m²/g. PCL nanofiber sheet was fabricated from the electrospinning method, including NP/SiO₂ dispersed in the surface of its thread by acoustic mixer. The samples were sampling the releasing of dye by decomposing PCL in PBS under 38°C at 100rpm inside incubator, then compute the degree of the amount of the dye release by UV-spectroscopy.

Wednesday, 21/Aug/2019 6:12pm - 6:24pm

Abstract ID: 347 / FCM: 12

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Design and application of composite structures

Keywords: Multiple-layer Coating, Buildings, Passive Cooling, Cooling Power, Energy Consumption

Developing a multiple-layer functional coating for buildings in hot and humid regions to achieve passive cooling and energy saving

Jianheng CHEN, Lin Lu, Hong Zhong, Yaxiong Ji

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A multiple-layer functional coating with high infrared emissivity, large reflection index of solar irradiance and good performance of reduction for heat conduction was newly developed to be applied on the surfaces of building roofs for achieving passive cooling and building energy saving. The multiple-layer consists of a SiO₂-TiO₂ composite layer for emitting radiation selectively within the atmospheric transparency window, an Ag layer for high solar irradiance reflection and a hollow glass microspheres layer for heat conduction insulation. A several of experimental chambers with or without the coating on the top surface were set up. Experiments were carried out simultaneously in Hong Kong to test the thermal behaviors of the chambers by measuring the varying inner chamber temperature and relevant cooling power. The spectral and thermal properties of each layer were measured and integrated into building numerical simulations for yearly building energy consumption to compare energy saving effects and roof surface temperature with or without the coating applied on the building roof. The experimental and simulation results present a promising applicability of the newly developed coating on building roofs for passively achieving energy saving and reducing severity of the urban heat island problem.

Thursday, 22/Aug/2019 9:30am - 9:42am

Abstract ID: 348 / FCM-2: 8

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Ceramic based composites

Keywords: Nanofibers, Graphene, Multi-gradient, Ceramic-based composite, Electrical conductivity

Multi-gradient electroconductive alumina

Irina Hussainova, Ali Saffarshamshirgar, Roman Ivanov

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Functional gradients are essentially featured by the creation of site-specific properties distributed within a material that originate from variations in such factors as composition, microstructure, geometry and entanglement combined with highly distinguished electrical and thermal properties of the constituents. Here we report a novel strategy to consolidate highly anisotropic multi-gradient alumina of excellent electrical conductivity in one direction and insulation in another one accompanied by gradient in grain size throughout the layers. The material was produced via incorporation of alumina nanofibers (10 ± 2 nm in diameter) decorated by several layers of graphene wrapped around a longitudinal axis of the fiber. The graphenated fibers, obtained with the help of one-step non-catalyzed CVD process, offered reinforcement combined with a high electrical conductivity of individual fiber for particulate alumina powders to be consolidated by spark plasma sintering (SPS). The SPS at 1350 °C in nitrogen atmosphere under 50 MPa pressure resulted in fully dense structures where the layers of relatively coarse grains of 1 – 3 μm in size were followed by the layers of fine grains of 0.05 – 0.2 μm through a thin transition layer. Gradient in mechanical properties ensured an increased indentation fracture toughness of the bulks. Gradient in electrical properties was achieved by gradual addition of the graphenated nanofibers into the matrix during a mold formation. The in-plane electrical conductivity of the specimen measured along the graphenated layer was 500 Sm^{-1} for an interlayer with 100 μm thickness and 15 vol.% of graphenated fibers. This value rises up to 1000 Sm^{-1} when the fibers fraction reaches 25 vol.% and up to 1700 Sm^{-1} by increasing the thickness of the layer to 500 μm . On the other hand, perpendicular to the layers the resistivity is no different from that of monolithic full-density alumina. Moreover, the thermal conductivity analysis revealed anisotropic thermal properties of the structure. Both contact and non-contact methods were used to determine the contribution of the enhancing hybrid layer and its interface with the monolithic alumina layer to the thermal conduction.

Abstract ID: 349

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Magnetic Nanomaterials for Applications

Keywords: Nanoflower, Hybrid Material, Magnetite Nanoparticles

Hybrid Magnetic Material for Removal and Reduction of Heavy Metals

Sajitha Sasidharan, Vivek Prakash, Vibin Ramakrishnan

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In the past few years a great deal of work has been dedicated in finding materials for removal and reduction of heavy metals from contaminated water. In our work we explored novel aromatic molecular systems, mediated through aromatic π - π interactions for such applications. The research work is categorized into two phases including (i) Synthesis and solvent assisted self-assembly of the novel trityl-based organic molecules into nanostructures (ii) Fabrication of nanostructures to hybrid materials for environmental applications. The new molecule 1, 2-bis(tritylthio)ethane synthesized and crystallized, self assembles into nanosheet like architecture, which further assembles to form a flower like morphology. A one-step process has been adapted to coat the assemblies with magnetite nanoparticles to form an organic – inorganic hybrid material. With the advantageous property of high surface area and hydrophobic nature of the hybrid material, the magnetic composite is used as an adsorbent for removing contaminants from water. The magnetic property of the material enables the subsequent control and removal of the product by simple magnetic separation. Enhanced removal of Cr was mainly attributed to higher specific surface area of the sheet and flower like morphologies, leading to more sites for the adsorption of magnetite and in turn Cr ions. The designed method is advantageous, as it reduces the heavy metals to non-toxic form with magnetite being the nanoadsorbent. The studies with this hybrid material can be extended to broad spectrum heavy metal removal. Our experimental results indicate that the designed method is advantageous as it is environment friendly, with no secondary pollutants, wide range pH stability, easy operational procedures and excellent adsorption capacity. The procedure mentioned not only addresses the key challenge faced in waste water treatment, but also based on the heavy metal ion trapped in the nano adsorbent, it delivers a potential nano-material for applications in diverse areas.

Abstract ID: 350

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Nanomaterials for Sensors, Flexible Electronics and Nanocomposites

Keywords: Tin oxide-based sensor, sol-gel synthesis, power transformer, carbon gases, gas-sensitive mechanism

Semiconductor gas sensor based on tin oxide on-line monitoring of dissolved gas in transformer fluids

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The power transformer is one of the most important devices in the transmission and distribution of electricity, so its operating conditions directly affect its safety and stability, and the failure of the transformer causes large losses for the operating company. Remote monitoring of a power transformer is becoming one of the most effective measures to improve safety and reliability. Monitoring of transformer insulation in the field becomes a necessary condition leading to the development of the power system, as well as a basic element of service. When a malfunction occurs inside the transformer, low molecular weight hydrocarbon gases, hydrogen, carbon monoxide and carbon dioxide dissolve in the transformer oil. In the present work, tin oxide-based sensors have been synthesized, and their sensitivity to carbon gases has been investigated. The molecular orbital energy of hydrocarbon gases was studied by the method of quantum chemical calculations and the existing gas-sensitive mechanism was qualitatively explained.

Thursday, 22/Aug/2019 12:30pm - 12:42pm

Abstract ID: 352 / FLNM-2: 8

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nanomaterials for Sensors, Flexible Electronics and Nanocomposites

Keywords: Copper and silver nanoparticles, Sensors, Electrically conductive fabrics, EMI shielding

Electrically conductive textile sensors made by silver and copper nanoparticles

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In this study, we make the electrically conductive multifunctional and durable textile sensors by silver and copper nanoparticles using a dipping– drying method. The fabric structure was pretreated with citric acid then nanoparticles were directly grown on fabric structure, hence absorbed by microfibers to form electrically conductive fibres. Particles filled the spaces between the microfibers, and were stacked together to form networks with high electrical conductivity. The effect of pretreatment was analyzed by FTIR. The dynamic light scattering, SEM and XRD techniques were employed to study the morphology of deposited silver and copper particles. The utility of conductive fabrics was analyzed for electromagnetic shielding ability over frequency range of 30 MHz to 1.5 GHz. The EMI shielding was found to increase with increase in concentration of particles. Furthermore, the role of deposited particles on antibacterial properties was examined against pathogenic bacteria such as Staphylococcus aureus and Escherichia coli. Moreover, effect of metal coating was observed against mechanical properties like tensile strength and crease recovery angle. At the end, the durability of coated fabrics for comfort and electrical properties were examined against several washing cycles. The fabrics showed good retention of the particles, proved by SEM microstructures and small loss in the conductivity of the material after washing.

Wednesday, 21/Aug/2019 5:48pm - 6:00pm

Abstract ID: 353 / FBB: 10

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biomaterials for musculoskeletal regenerative engineering

Keywords: Nanopattern, RGD, MSC, chondrogenesis, tenogenesis

Nanopatterned substrates to promote chondrogenesis and tenogenesis in mesenchymal stem cells

Ignasi Casanellas^{1,2}, Anna Lagunas^{3,1}, Sergi Casanova^{1,2}, Yolanda Vida^{4,5}, Ezequiel Pérez-Inestrosa^{4,5}, Cristina Rodríguez-Pereira⁶, Joana Magalhaes^{3,6}, José A. Andrades^{7,3}, José Becerra^{7,3,5}, Josep Samitier^{1,3,2}

¹Institute for Bioengineering of Catalonia (IBEC), Barcelona Institute of Science and Technology (BIST), Spain; ²Department of Electronics and Biomedical Engineering, University of Barcelona, Spain; ³Networking Biomedical Research Center (CIBER), Madrid, Spain;

⁴Instituto de Investigación Biomédica de Málaga (IBIMA), Department of Organic Chemistry, Universidad de Málaga (UMA), Spain; ⁵Andalusian Centre for Nanomedicine and Biotechnology-BIONAND, Málaga, Spain; ⁶Unidad de Bioingeniería Tisular y Terapia Celular (GBTTC-CHUAC), Instituto de Investigación Biomédica de A Coruña (INIBIC), Complejo Hospitalario Universitario de A Coruña (CHUAC), Sergas, Universidade da Coruña (UDC), Spain; ⁷Instituto de Investigación Biomédica de Málaga (IBIMA), Department of Cell Biology, Genetics and Physiology, Universidad de Málaga (UMA), Spain; icasanellas@ibecbarcelona.eu

Cell adhesion and differentiation processes are influenced by nanoscale cues of the extracellular matrix (ECM), being more affected by its local rather than global disposition. We have developed a method to produce large-scale substrates nanopatterned with cell-adhesive moieties of arginine-glycine-aspartate (RGD) dendrimers (1). The method presented here is very simple and can be extended to other ligands having density effects on cells.

Cartilage and tendon lesions and degeneration are frequent. Their poor ability to self-repair has fostered the development of stem cell-based strategies; however, current procedures still fail to reproduce the functional tissue architecture.

We have previously shown that RGD dendrimer nanopatterns can be tuned to promote chondrogenesis. By adjusting local ligand density at the nanoscale, we modulated the initial stages of cell condensation and differentiation (2, 3). Cartilage being an avascular tissue, the establishment of a gap junction intercellular communication (GJIC) network during formation is crucial for the final tissue homeostasis. We here demonstrate that nanopatterns also promote GJIC in the developing cartilage, an indicator of improved tissue functionality.

Nanopatterned substrates were combined with mechanical loading stimuli to guide differentiating MSCs towards the tenogenic fate, while still providing the structural cues required for effective tendon regeneration.

This study provides new insight into nanoscale cell-matrix interactions in the early stages of cell differentiation. The developed technology will contribute towards new stem cell-based regenerative therapies of cartilage and tendon.

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Abstract ID: 354

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

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

Keywords: Colloidal nanoparticles, Capillarity, Two-dimensional monolayer, Optical detection, Liquid interface

Pinpoint Deposition of Nanoparticle Monolayer on Various Solid Substrates without Considering Surface Chemistry

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Deposition of two-dimensional arrays of closely packed plasmonic nanoparticles is a promising technique for optical detection of molecules on solid surfaces due to high signal enhancement associated with their multiple hotspots over a large area. However, a reproducible deposition of uniform nanoparticle layers on various solid surfaces is highly limited by the surface energy and topography of the solid surface, thus making practical biological and chemical sensing challenging. Here, we propose a facile and direct method to build on-demand Raman sensors on generic solid substrates by selective transfer of interfacial nanoparticle monolayers using a simple capillary tube. First, nanoparticles are forced to be self-organized into nanoparticle monolayer at water/air interface. The small portion of the nanoparticle monolayer at the interface is selectively separated by a capillary tube due to a capillary rise. Then, the tube is reversed upside-down to expose the monolayer to the other end of the tube. The exposed monolayer is finally transferred to solid substrates without any adhesion to the capillary sidewall. Our method enables the pinpoint placement of various nanoparticle monolayers at target locations of solid substrates regardless of their surface geometry. Finally, we successfully extend our method to the surface of various products that are commercially available for practical chemical sensing applications.

Wednesday, 21/Aug/2019 4:39pm - 4:51pm

Abstract ID: 355 / FC: 4

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Green catalysis

Keywords: Mechanochemical, ball-milling, composites, catalysis, oxidation

Simple solvent-free preparation of heterometallic composites and their applications in catalysis

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Preparation, characterization and application of dispersed materials and composites with high surface-to-volume ratio constitute one of the important directions of modern chemistry and technology. Thus, engineering simplification and cost efficiency can be indicated as targets to pursue for the wide introduction of nano- and similar technologies into practice. In this view, mechanochemical and similar dry synthetic methods can be particularly interesting since they can exclude solvation and surface effects, which can significantly influence and hinder the preparation of new dispersed materials at nano- and micro-scale.

The application of a simple, time- and energy-saving mechanochemical ball-milling synthetic procedure for the preparation of multifunctional dispersed materials, using cheap and available starting materials is reported. The prepared heterometallic dispersed composites are screened for the peroxidative oxidation of alcohols and alkanes, under mild conditions. Several parameters such as size, type and number of milling balls, reaction time (milling time) are evaluated. The influence of multiwalled carbon nanotubes (CNTs) and graphene oxide (GO) as additives are tested towards the optimization of the catalytic processes. A comparison with traditional wet synthetic approaches will be discussed to highlight advantages of mechanochemistry and its high energy efficiency.

Thursday, 22/Aug/2019 2:39pm - 2:51pm

Abstract ID: 356 / FCM-4: 4

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Metal matrix composites

Keywords: MMC layers, Laser surface alloying, Copper, Diode laser, Microstructure, Wear resistance

Microstructure and properties of copper matrix composites fabricated by laser surface alloying

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Metal matrix composite (MMC) surface layers reinforced by WC+Cr particles were fabricated on copper by a laser surface alloying process. WC+Cr - reinforced composite surface layers on a copper substrate were carried out using a High Power Diode Laser. Laser surface alloying techniques have received much attention as an alternative to more conventional techniques for fabricating MMC. During the laser surface alloying process the powder mixture, together with a thin surface layer of the substrate, is melted using a laser beam. This leads to rapid solidification and formation of composite surface layer.

The microstructure, chemical composition and phase composition of the MMC surface layers were studied by means of scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), and X-ray diffraction (XRD) techniques. Rietveld refinements for obtained patterns were made in order to assess the unit cell parameters of phases in the composite surface layer. WC+Cr particles were dispersed uniformly in MMC layers. The increased hardness of the surface layer of copper after the laser alloying with WC+Cr particles is a result of solution hardening, dispersion hardening and the grain refining. Laser alloying of copper enables the production of wear-resistant composite surface layer with high tribological properties. The composite surface layer properties tend to be improved to those of the untreated copper base material.

Abstract ID: 357 / Poster: 7

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Advances in the Synthesis and Characterization of low dimensional, nano and 2D materials

Keywords: Carbon nanotubes, Nanowires, Raman spectroscopy, DFT calculations

Raman spectroscopy characterization of ultrathin metal-chalcogenide and metal-halide nanowires encapsulated in single-walled carbon nanotubes – theory and experiment

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Single-walled carbon nanotubes (SWCNT) serve as an effective template for one-dimensional (1D) crystallization of nanowires of diverse chemical compositions [1,2]. The nanowire@SWCNT composites are subject of extensive research for their structural, electronic and optical properties. For example, the charge transfer between the SWCNT and the encapsulated material may result in a p- or n-type doping of the surrounding nanotube, thus inferring for application of such materials in nano- and optoelectronics. In this aspect, the development of fast and reliable methods for characterization of encapsulated 1D crystals is a hot topic in the modern material science. Here we report on the advances of Raman spectroscopy as a sensitive probe for ultrathin MX@SWCNT nanowires (M = metal and X = S, Se, Te or Cl, Br, I). Many of the bulk MX chalcogenides and halides do not possess Raman activity. The lateral confinement of the corresponding materials on a sub-nanometric scale, however, leads to the appearance of several Raman-allowed modes [3,4]. The comparison between the predictive DFT calculations and the experimentally recorded Raman spectra of the MX@SWCNT composites allow to identify the chemical composition and the diameter of the encapsulated nanowires. In particular, it has been established for 2×2 and 3×3 HgTe@SWCNT and KI@SWCNT composites that the strongest Raman modes comprise of radial breathing motion (RBM) of the encapsulated nanowires.

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Thursday, 22/Aug/2019 4:03pm - 4:15pm

Abstract ID: 358 / FESC-2: 11

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: Magnetic Nanoparticles, Negative electrode, magnetization

Carbon modified Iron oxide magnetic nanoparticles - negative electrode material for supercapacitor applications

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Carbon modified metal oxide has been established as a suitable electrode material for supercapacitor applications. Especially the opportunities on iron oxide is motivated the current researchers due to the theoretical specific capacitance value for Fe₃O₄ and Fe₂O₃ were 2606 and 3625 F/g which is too large compared to present electrode materials [1-2]. Based on the present challenges such as their low cycling stability, we have developed carbon modified octahedral shaped magnetic nanoparticles as a negative electrode material. Iron oxide nanoparticles were prepared by chemical oxidation method [3] and carbon modification was achieved using sugar solutions. XRD, FESEM and TEM analysis were used to study the structural and morphological characteristics. Magnetic characteristics of the carbon modified octahedral shaped iron oxide nanoparticles were analyzed using VSM. Bare and carbon modified iron oxide magnetic nanoparticles showed the saturation magnetization of 90 and 87 emu/g. Figure 1 shows the TEM micrograph of bare and carbon modified Fe₃O₄ magnetic nanoparticles. Carbon modified iron oxide has been utilized as a negative electrode material and showed a specific capacitance of 274 F/g with a stability of above 80 % retention even after 5000 cycles.

Thursday, 22/Aug/2019 11:24am - 11:36am

Abstract ID: 359 / FTF: 3

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Sol-gel and LB technology

Keywords: SiO₂, thin films, barrier coatings, high pressure vessels

Organically functionalized sol-gel silica coatings on polymers for reduction of gas leakage

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The problem of gas leakage is closely related to the high pressure storage of gases – especially hydrogen, which have a high potential to be used as eco-friendly fuel but also permeate easily through all types of materials due to its molecule size and properties. Our idea concerns the reduction of gas permeability through polymeric materials, which constitute the liner of currently developing high pressure vessels – type IV. The received silica coatings were functionalized with organic groups in a way to provide the best integration of coating with the liner. The coatings modified with different functional groups were obtained by the unconventional sol-gel process – without added water – and applied on polymeric substrates by dip-coating method. In order to increase the adhesion of coatings to the polymeric material, characterized by low surface free energy, the surface of substrates was successfully activated immediately prior to the first layer application process by UV-ozone treatment. The obtained layers were characterized by continuity and relatively high density, what promotes the use them as the gas barrier coatings. The functionalization caused changing the silica network structure what influenced properties of received coatings, especially a mechanical parameters, what in result should allow to obtain coatings working well with the tank during fueling and refueling process. To determine mechanical behavior of coatings scratch tests and tensile tests connected with microscopic visualizations were conducted. Physicochemical measurements – microscopic and composition analysis – were carried out to characterize the morphology and topography of obtained coatings. The barrier properties were determined by the permeability measurements and the permeability and permeability coefficient were calculated for different gases. This study presents range of possible organically modified silica sol-gel coatings with different application properties, which can be adjusted to selected purposes, with emphasis on gas barrier, even for hydrogen.

Thursday, 22/Aug/2019 2:36pm - 2:48pm

Abstract ID: 360 / FTF-2: 4

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Structure Formation in Multi-Component thin films

Keywords: thin-film processing, evaporation, condensation, phase separation, organic electronics

Structuring polymer solutions upon liquid-vapor mass exchange

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Organic and hybrid thin film electronic devices, such as memory diodes, solar cells and transistors, typically contain a functional layer based on a blend of multiple polymeric or small-molecular species whose properties cooperatively give rise to a specific function. Depending on the desired functionality, phase separation during thin film solution processing is either encouraged or suppressed. Usually, at least one blend component is polymeric, so that mutual repulsion readily overcomes the entropic driving force to form stable mixtures. For this reason, it is often observed that during solution-casting droplet-like demixed morphologies emerge due to (spontaneous) liquid-liquid (L-L) demixing. This presentation focuses on the role of this mode of phase separation in thin film electronics and how it is induced by mass exchange across the liquid-vapor boundary, i.e. solvent evaporation and vapor condensation. I give an overview on the work we have done to theoretically understand the influence of liquid-vapor exchange rates on demixing kinetics, as well as domain structure and composition. Multi-component continuum limit modeling demonstrates how microstructure and feature sizes emerge upon solvent evaporation and/or vapor condensation. The numerical simulations yield morphologies consistent with experimentally observed structures and demonstrate how domain size and phase composition are affected by internal and environmental factors.

Abstract ID: 361 / Poster: 2

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Nanostructured Precious Metals

Keywords: urchin-like gold mesostructure, SERS substrate, cellulose nanocrystal, nanothorn

Biocellulose Nanocrystal-Assisted Fabrication of Uniform Urchin-like Gold Film for Using as SERS Substrate

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Surface-enhanced Raman scattering (SERS) with high enhancement, reproducible signal, and long-shelf-life is essential for practical applications in identification of trace chemicals and recognition of molecular fingerprint of biomolecules. In this paper, we develop a simple approach for the fabrication of desirable SERS substrate consisting of urchin-like gold mesostructure (UL-AuMS) uniformly deposited on a rough surface of bacterial cellulose nanocrystal (BCN) film. A circular film of BCN (ca. 1.5 mm diameter and 50 μ m thickness) was solvent casted on a polydimethylsiloxane (PDMS) film from a 2- μ L drop of BNC colloid before drying at 100 $^{\circ}$ C for 10 min. The rough surface of BNC film with abundant hydroxy groups became anchor points for UL-AuMS. Uniform UL-AuMSs (638 \pm 12 particle size with 398 \pm 7 core size and 214 \pm 19 nanothorn length) were synthesized by our green chemistry approach using hydrogen peroxide as a reducing agent and silver nitrate as a shape-controlling agent. A 2- μ L suspension of UL-AuMSs was deposited on the BNC film. UL-AuMSs uniformly deposited on the opaque white BNC film and turned its color to slight golden-white. The density of UL-AuMS on BNC film can be tuned by adjusting the concentration of the suspension. The UL-AuMS film shows excellent SERS enhancement due to its inherent sharp tips and small cavity. The packing density is expected to play a key role in SERS enhancement. Our fabricated SERS substrate is very economical since only 3.2 μ g of gold metal was deposited on the BNC film.

Abstract ID: 362

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin films for optoelectronics, nanoelectronics and spintronics

Keywords: nanoparticles, polymer blending, semiconductor, light-emission

Polymer light-emitting diodes with an emitting layer based on a nano-confined semiconducting polymer blend

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Blending a visible light-emitting organic semiconductor with an insulator alleviates the trap-limited nature of the electron current. Organic light emitting diodes (OLEDs) comprising such a blend as emissive layer exhibit a two-fold increase in luminous efficiency with only 10% semiconductor. Due to this low content of semiconductor, polymer-LEDs are more attractive than small molecule-based devices. However, polymers impose the difficulty of an inherently low miscibility. In a plain blend macro-phase separation can be avoided if the molecular weight is kept low, which, in case of the semiconductor, is a disadvantage as it suppresses charge carrier mobility. An alternative strategy is to impose a nano-confinement. We prepare aqueous nanodispersions of red (PPV) and blue (polyfluorene) emitting polymers, blended with polystyrene as insulator. We seem to fully suppress macro-phase separation in both cases. For the latter, the combination of nano-confinement and blending influences the phase morphology of the semiconductor in an unprecedented way. Fabricating OLEDs with an emitting layer consisting of nanoparticles poses a considerable challenge due to high operational current densities. We now succeed in fabricating such devices in a reproducible way at very decent efficiencies.

Abstract ID: 363

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC) Oral Presentation

Topics: Solar Cells

Keywords: Perovskite solar cell, organic semiconductors, electron transport layer, interface passivation

Interface Tuning in Solution processed Organic and Hybrid Perovskite Solar Cells

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Hybrid organo-metal halide perovskite solar cells (PSCs) and organic polymer solar cells (OPVs) are two of the most promising candidates for next generation photovoltaic device primarily due to their high efficiency, printability and low cost.

Interface Engineering has played significant role in advancing the organic polymer solar cell technology, including inverted solar cell structure, tandem polymer solar cells etc.[1] Many of the know-hows have also been successfully applied in hybrid perovskite solar cell research. In this talk, the following two topics will be presented:

(a) perovskite/HTL interface tuning - As perovskite is very humid sensitive, we are interested in exploring the application of hydrophobic organic semiconductors in PSCs. We incorporated (a) non-fullerene acceptor, and (b) p-type π -conjugated polymer (PBDB-T) into the anti-solvent process of perovskite film formation. [2],[3] The organic semiconductors effectively passivate the trap states of the mixed perovskite film, for example, through the formation of Lewis adducts between lead and oxygen atom in PBDB-T. The process improves charge-transport, and the hydrophobic NFA molecule and PBDB-T prevent moisture invasion into the perovskite active layers. This leads to high-efficiency ~20%, and significantly improved device stability

(b) Metal oxide electron transport materials – (i) a facile yet effective two-step method, i.e., room-temperature colloidal synthesis and low-temperature removal of additive (thiourea), to control the size (3 – 5 nm diameter) and carrier concentration of SnO₂ quantum dot (QD) ETLs to achieve high performance PSCs. By optimizing the electron density of SnO₂ QD ETLs, we are able to achieve a champion reverse scan PCE of 20.8%, stabilized power output (SPO) of 20.32% for the planar PSCs using triple cation perovskite absorber (Cs_{0.05}(MA_{0.17}FA_{0.83})_{0.95}Pb(I_{0.83}Br_{0.17})₃) (MA = CH₃NH₃, FA = HC(NH₂)₂) and 19.73% for those using CH₃NH₃PbI₃ absorber. (ii) Solution process, chemically pure tin oxide nanoparticles via physical ball-milling approach and its application as electron transport layer in perovskite solar cells was investigated. [5]

Key Words: Perovskite solar cell, organic semiconductors, electron transport layer, interface passivation

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Abstract ID: 364

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Advances in Deposition Techniques for thin films

Keywords: PP filter, Biomass, Nano coating, Pure water

Nano Surface Coating of Pure Water PP Sediment Filter by P.V.D method to Reduce Biomass Affection

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Biomass growth and bio-fouling within pure water systems present potentially serious problems. High filtering efficiency that can remove dirt, rust, dust, silt, algae and the other, could not prevent bacterial growth to reduce harmful bacteria and microorganisms unless being coated by some disinfectant nano coating materials like silver. Physical vapor deposition (P.V.D), as a special technique used to coat a thin layer of nano silver on the PP Sediment filter surface. So It improves the PP sediment filter application with the 40 nm silver coating thickness in specific temperature (up to ten degree more than 25 oc) in 0.1 nm/sec evaporation rate and 3×10^{-5} Torr vacuum condition. The multi-layers of PP sediment filter tissue of polypropylene yarn are full of fine pores that can be decreased by nano materials coating. In this way, the biomass affection declines because of both the filter pore size reduction and the anti-microbial nano silver thin layer. Scanning Electron Microscopy (SEM) technique helped to compare the polypropylene filters images in arbitrary magnitudes. The results of bacterial testing on pure water samples show the nano silver coated effects successfully.

Wednesday, 21/Aug/2019 5:03pm - 5:15pm

Abstract ID: 365 / FC: 6

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Photocatalysis

Keywords: Photocatalysis, CO₂ reduction, DFT simulations

Silicon Nanoparticles-based Photocatalysts for Efficient CO₂ Reduction

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Solar-driven hydrogenation of CO₂ to chemical fuels and value-added products is emerging as an excellent source of renewable energy for future; and has potential for operating at industrial scales, while reducing the detrimental effects of greenhouse emissions. However, the best performing catalysts for photocatalytic CO₂ reduction are still made of rare and expensive elements such as platinum or palladium. In this work, we will present the progress on the development of new photocatalysts made of silicon, an earth-abundant and relatively inexpensive element. Our focus in this talk will be on elucidating fundamental reaction mechanisms and improvement strategies, using density functional theory (DFT) and ab-initio molecular dynamics simulations. First, we will report on hydride-terminated silicon nanocrystals that can function as a single component heterogeneous reducing agent for converting gaseous carbon dioxide selectively to carbon monoxide, at a rate of hundreds of $\mu\text{mol h}^{-1} \text{g}^{-1}$ owing to their large surface area, broadband visible to near infrared light harvesting and reversible reaction mechanism¹. Next, we will discuss enhancing this catalyst activity by supporting this silicon photonic crystal by ruthenium, which results into CO₂ reduction rates as large as 2.8 mmol h⁻¹ g⁻¹ at ambient temperature; and the corresponding atomistic mechanism underpinning this reaction². The results from the DFT simulations indicate that charged Ru surfaces can destabilize adsorbed CO₂ molecules and adsorb and dissociate H₂ such that it can readily react with CO₂, thereby accelerating the Sabatier reaction. Overall, this work will highlight the strategies for developing and utilizing nanostructured hybrid catalysts for efficient reduction of gaseous carbon dioxide to chemical fuels directly from sunlight.

Thursday, 22/Aug/2019 8:48am - 9:00am

Abstract ID: 366 / FLNM: 5

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nanomechanics

Keywords: graphene, strength, Raman mapping, cracks

The Strength of Mechanically-Exfoliated Monolayer Graphene

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The deformation and fracture behaviour of one-atom-thick mechanically exfoliated graphene has been studied in detail. Monolayer graphene flakes with different lengths, widths and shapes were successfully prepared by mechanical exfoliation and deposited onto poly(methyl methacrylate) (PMMA) beams. The fracture behaviour of the monolayer graphene was followed by deforming the PMMA beams. Through in-situ Raman mapping at different strain levels, the distributions of strain over the graphene flakes were determined from the shift of the graphene Raman 2D band. The failure mechanisms of the exfoliated graphene crystals were either by flake fracture or failure of the graphene/polymer interface. The fracture of the flakes was observed from the formation of cracks identified from the appearance of lines of zero strain in the strain contour mapping graphs. It was found that the strength of the monolayer graphene flakes decreased with increasing flake width. The strength dropped to only ~ 5 GPa for large flakes, much less than the reported value for monolayer graphene of 130 GPa, thought to be due to the presence of defects in the crystals. It is shown that a pair of topological defects in monolayer graphene will form a pseudo crack and the effect of such defects upon the strength of monolayer graphene has been modelled using density functional theory.

Abstract ID: 367

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nanomaterials for Sensors, Flexible Electronics and Nanocomposites

Keywords: silver acetate, silver nanoparticles, porous silver film, sintering, thermal decomposition

Fabrication of porous silver film by thermal decomposition of rod shape silver acetate under a suppressed sintering of nanoparticles

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In this research, a simple and low-cost synthetic protocol for fabricating porous silver film by a thermal decomposition of rod-shaped silver acetate (RS-AcOAg) was developed. RS-AcOAg was synthesized directly from silver granules via our green chemistry approach. A solvent-cast thin film of randomly stack RS-AcOAg turned into a sponge-like silver film after a thermal treatment at 280°C for 15 min. The thermal treatment induced the formation of silver nanoparticles (AgNPs) on the surface of RS-AcOAg with the expense of RS-AcOAg rod. AgNPs sintered into bigger particles while turning RS-AcOAg film into a silver film consisting of interconnected quasi-sphere silver microparticles (particle size of 300-500 nm). The sintering decreased the surface area of the film while limiting its potential applications. To suppress the sintering of the thermally generated AgNPs, liquid polydimethylsiloxane (IPDMS) was coated on the surface of RS-AcOAg rod before the thermal treatment. The thermally stable IPDMS thin film inhibited the mobility of AgNPs and suppressed the sintering. As a result, the porous silver film consisting of interconnected AgNPs (particle size of 100-140 nm) was obtained. The morphology and porosity of the porous film can be manipulated via the loading of IPDMS. The porous silver film with IPDMS-suppressed sintering has potential applications as a catalyst, surface enhanced Raman scattering (SERS) substrate, conductive filter, and conductive flexible circuit.

Abstract ID: 368

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Metal oxide, carbon, nitrides etc based thins Films

Keywords: Nitridation, Metallic Grating, Tube, Plasmonic Excitation

Nitridation of a TiO₂ based sol-gel diffraction grating to a metal-like TiN-based plasmonic grating extended in tubular geometries

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Within this study, we demonstrate the conversion of a pure dielectric planar TiO₂ solgel diffraction grating to metallic one by means of ammonolysis. In particular, a micro structured TiO₂ sol-gel grating printed on a silicon substrate is transformed into a metallic non-stoichiometric TiO_xNy quasi-sinusoidal grating. Initially, a non-structured TiO₂ layer is photo-patterned by a UV linear polarized beam through a chromium photo-mask grating using the negative properties of the TiO₂ solgel layer. To attain nitridation, the xerogel TiO₂ grating undergoes a heat treatment under Ar gas and a following constant NH₃ flow enabling the modifications of the micro structured TiO₂ grating to a TiO_xNy grating according the amonolyse process. This process returns a metallic grating that sustains plasmonic effects in the near infrared bandwidth revealed by the investigation of the optical properties of the derived TiO_xNy grating [1]. Additional experiments exhibit a material with an adequate hardness, a good chemical stability and low loss against the classical metals rendering it an attractive candidature for numerous technological functions.

Such an infinite grating can be subjected to the holistic phenomenon that permits the planar to cylindrical grating rolling conserving the same number of grooves without any overlap. To this orientation, a novel structuration has conceived which endorses a TiO₂ solgel based diffraction grating in the walls of a silica tube [2]. The fabrication of the grating is realized with a radial phase mask, which transforms optically a 2D planar ring grating to a 3D periodical structure in the tube cavity projecting the ± 1 TE orders in air by a single step exposure. The objectives are to transfer previous results on planar substrates to perform metallic grating by means of ammonolysis process inside the wall of an 8 mm diameter tube from a TiO₂ based grating. From expected results concern holistic plasmonic excitation in TiO_xNy – grating in air interface with a resonance in the NIR range.

Abstract ID: 369

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Drug delivery/controlled release

Keywords: ZnO nanoparticles, Poly ethylene glycol, Tetracycline, wet chemical precipitation

Poly (ethylene glycol)-coated zinc oxide Nanoparticles as carriers for topical delivery of tetracycline

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In the past two decades, zinc oxide nanoparticles have become one of the most popular metal oxide nanoparticles in topical drug delivery due to their excellent biocompatibility, economic, and low toxicity. But when these materials are used in aqueous solutions, an accumulation of them have been observed. Poly ethylene glycol (PEG), showed steric effects which would help to stabilize the nanoparticles preventing them from agglomeration or dispersion in solutions. In this contribution we tried to improve the stability of drug loaded-ZnO nanoparticles and controlled release of drug loaded ZnO nanoparticles using PEGylation technique. Tetracycline was used as a model drug. ZnO nanoparticles were prepared by wet chemical precipitation method and characterized by scanning electron microscope, Fourier transform infrared spectrum, X-ray photoelectron spectrum, and dynamic light scattering techniques. Tetracycline was loaded to these ZnO nanoparticles in different drug/ZnO ratios and their surface were coated with poly ethylene glycol (PEG) in order to improve their biological stability and controlled drug release. The results indicates a high stability and a sustained release pattern of tetracycline from PEG-coated ZnO nanoparticles. Additionally, the ex vivo permeation through human skin study using vertical Franz diffusion cells revealed higher permeation for tetracycline from these nanoparticles when compared with the aqueous solution of the drug.

Thursday, 22/Aug/2019 12:48pm - 1:00pm

Abstract ID: 370 / FTF: 10

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Advances in Deposition Techniques for thin films

Keywords: Supported Lipid Bilayer, Roll to roll processing, Directed Self-Assembly

Roll-to-roll processing of supported lipid bilayers: flexible substrates, rapid-prototyped inking, and shippable membranes

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Supported lipid bilayers are self-limiting, molecularly thin fluid films which can be readily biofunctionalized. Their utility is traditionally limited by their delicate, non-scalable fabrication methods. We have addressed the major challenges to producing supported lipid bilayers on industrial scales via roll to roll processing. These include characterizing a low cost lipid-compatible flexible substrate, prescribing continuous lipid inking patterns via rapid prototyping, and a surface processing methodology that enables shippable films for on-site membrane formation. The directed self-assembly approach is based on lipid surface spreading, where surface-adhering bilayers project geometrically from lipid stacks. The resulting systems can be designed either as large continuous membranes or as discrete, dynamic patterns.

Thursday, 22/Aug/2019 9:00am - 9:12am

Abstract ID: 371 / FLNM: 6

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

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

Keywords: 1D/2D nano/micro material, 3D integration, Room temperature transfer printing

Room-temperature 3D integration of low-dimensional nano and 2D materials on flexible substrates by transfer printing methods

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The 3D integration of one-dimensional (1D) or two-dimensional (2D) nanostructures onto the flexible substrates has the potential to offer significant performance gains to flexible electronic devices due to high integration density, large surface area, controllable surface energy, and improved light absorption and trapping [1,2]. We developed a simple, rapid and room temperature transfer printing methods with ultrasonic vibration and UV adhesive for this purpose. Uniformly interconnected 2D nano/micromesh structures ((CuNi, CuMg, AgNi, Ni etc.)) on diverse flexible substrates (Polyethersulfone (PES), Polyimide (PI), Polyethylene terephthalate (PET) etc.) were fabricated using room temperature transfer printing method. In addition, ultrasonic vibration was used to achieve room temperature transfer bonding of 1D materials (silicon nanowires (SiNWs etc.)) from their mother substrate to 2D structures on a flexible substrate (graphene/PET) within a few seconds. The microscopic structure and mechanical and electrical characteristics of the interface between 1D or 2D nanostructures and the flexible substrates were subsequently investigated, revealing that this creates a mechanically and electrically robust contact. We also applied these structures for flexible transparent heater and gas sensor. Therefore, it is considered as a valuable technique for integrating 1D or 2D nano/micro-structures onto the flexible substrates for flexible photovoltaics, energy storage, water splitting systems, polymerase chain reaction (PCR) systems, defogging/deicing systems, and particulate matter (PM) detecting systems.

Abstract ID: 372 / Poster: 18

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Applications of Composites

Keywords: Titanium dioxide, nanocomposite, biopolymer, ethylene scavenger, papaya fruit.

Development and characterization of HPMC-TiO₂ and Gelatin- TiO₂ nanocomposites as ethylene scavengers for climacteric fruit application

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Titanium dioxide (TiO₂) photocatalytic nanoparticles, nontoxic, an inert oxide, have been investigated as antibacterial agent and ethylene scavenger to extend the shelf life of packaged fresh fruit, especially climacteric fruits as papaya (*Carica papaya* L) [1]. However, TiO₂ suspended nanoparticles have a limited application due to their larger tendency to agglomeration, especially at high concentrations. It causes the scattering of incident UV light, decreasing the photocatalytic efficiency of TiO₂ [2]. This research aims to develop nanocomposite based on TiO₂ and hydroxypropyl methylcellulose (HPMC-TiO₂) and TiO₂ and bovine gelatin (Gelatin-TiO₂) for covering polyethylene packages used to protect fruit against injuries. It was investigated the effects of TiO₂ concentration (0,0.5, 1 and 2% w/w, i.e, related to polymer mass) and biopolymer matrix type on physicochemical, morphological, crystallinity, optical, thermal, mechanical, gas permeability and photocatalytic properties of nanocomposite films prepared by casting technique. Preliminary results suggested that polymeric matrices were able to disperse TiO₂ nanoparticles and crystallinity, chemical composition, thermal and optical properties were changed by the incorporation of TiO₂ into polymer matrices. However, thickness, moisture content and hydrophilicity of HPMC and gelatin-based films did not change by the increasing of TiO₂ concentration. Studies about mechanical and gas permeability properties, photocatalytic activity of nanocomposites as ethylene scavengers for papaya fruit as well as properties of polyethylene packages covered by nanocomposites will be investigated.

Abstract ID: 373 / Poster: 19

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Applications of Composites

Keywords: active packaging, food technology, nanotechnology, postharvest, papaya golden

Antimicrobial activity and ethylene scavenging of food packaging based on hydroxypropyl methylcellulose and silver nanoparticles

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Papaya (*Carica papaya* L.) is a crop of great economic importance worldwide, this fruit is consumed fresh in many countries and has a high potential to be industrialized. Brazil is one of the world's largest producers of papaya, particularly, papaya var. Golden. Postharvest losses caused by fungal pathogens such as *Colletotrichum gloeosporioides* as well as rapid maturation due to the ethylene production represent factors limiting papaya useful life [1]. Active packaging which can inhibit microbial growth and prevent the negative effect of ethylene is desirable to extend the shelf life of papaya fruit. Silver nanoparticles (AgNPs) are materials with antimicrobial activity and not well-known ethylene scavenging properties [2, 3]. The aim of this research is study the effect of silver nanoparticle concentration (0, 0.2, 0.5 and 2% w/w) on some physicochemical and morphological properties of hydroxypropyl methylcellulose (HPMC) films produced by casting technique as well its potential application to reduce fungal growth and ethylene production in papaya fruit var. Golden. Preliminary results suggest that color and surface hydrophilicity of HPMC films were significantly modified with the increase of the concentration of AgNPs. In contrast, moisture content and thickness were not altered with AgNPs concentration. HPMC films containing AgNPs inhibited the fungal growth on papaya surface. Complementary studies will be carried out to characterize the effect of AgNPs on the morphology, chemical, structural, water vapor permeability and mechanical properties of HPMC films. Also, the effect of AgNPs concentration on the ethylene scavenging in papaya fruit as well as the migration of components from the nanostructured films will be investigated.

Wednesday, 21/Aug/2019 4:48pm - 5:00pm

Abstract ID: 374 / FCM: 5

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: composite, simultaneous, pollutants

Nanocomposite WO₃-TiO₂ /fly ash with dual functionality in simultaneous removal of pollutants from wastewater

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The main problem related to effluents resulted from the textile industry is the colour that reduces light permeability, thus leading to a negative impact on photosynthesis. Other pollutants that result from this industry are heavy metals from dyes and surfactants used as additives. Wastewaters with a complex load like these must be treated before discharge. Several methods are used, among these are: chemical precipitation, coagulation, flocculation, membrane filtration, reverse ion-exchange osmosis, photodegradation and adsorption. The individual WO₃ and TiO₂ nanocrystals were obtained either by sol-gel. The TiO₂ and WO₃ powders were added during the hydrothermal treatment that was carried out in a stainless steel autoclave under constant temperature. The new composite material was characterized in terms of crystallinity (XRD) and surface properties: morphology (SEM, AFM), wettability (contact angle measurements), specific surface (BET) and FT-IR. During the hydrothermal processing large agglomerates are formed, as confirmed by the SEM images. However, the AFM images show that a regulate surface was obtained with an average roughness of 8.97 nm. The adsorption capacity was tested on mono- and multi-pollutants systems containing two dyes: Bemacid Blau and Bemacid Rot and one heavy metal ion-Cu²⁺. The optimized process conditions were identified. The initial and residual dye concentrations in the aqueous solution was analyzed by UV-VIS spectrometry (Perkin Elmer Lambda 25), while the heavy metal concentration was analyzed by AAS (Analytic Jena, ZEE nit 700), at $\lambda_{Cu} = 324.75\text{nm}$, respectively. The adsorption parameters (contact time, amount of substrate and initial concentration of the pollutants) were optimized for obtaining a maximum efficiency and were further used in thermodynamic and kinetic studies, comparatively discussed with the photocatalysis optimized operating parameters. The VIS- photocatalytic properties of the composite material were evaluated in pollutants systems containing one, two or three pollutants (Cu²⁺⁺BB+BR). During the photodegradation experiments some parameters such as contact time, the amount of substrate and the initial concentration of the pollutants were optimized. They were further used in thermodynamic and kinetic studies. The kinetic studies indicate that the adsorption of all the three pollutants follows the pseudo-second order equation. A new composite material obtained using fly ash, TiO₂ and WO₃ is active under VIS irradiation, proves good efficiencies in the simultaneous removal of dyes (BB, BR) and heavy metal (Cu²⁺). The adsorption and photocatalysis results obtained in static regime represent a starting point for continuous flow processes.

Abstract ID: 375

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Ni-Cu-Zn ferrites, Atomic dopants, Combustion temperature, Magnetic properties.

Spinel Ferrites with different Combustion Temperature: A comparison study of Structural and Magnetic Properties

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Ferrites are one of the most important sets of magnetic materials which have vast applications in technology and industry. Physical properties of ferrites strongly depend on their microstructure including crystal structure, atomic dopants, particle size etc. also it is well known that the microstructural characteristics directly depend on the fabrication method. Here, for the first time, we have investigated the effect of combustion temperature in auto-combustion preparation of spinel ferrites on the properties of them including microstructure and magnetic properties. Our findings show that by controlling the combustion temperature one can control the degree of crystallinity and in turn magnetic properties of spinel ferrites. Two sets of $\text{Ni}_{0.8-x}\text{Cu}_x\text{Zn}_{0.2}\text{Fe}_2\text{O}_4$ ($x = 0.2, 0.4, 0.6$) ferrite samples are fabricated using auto-combustion method at two different combustion temperatures of 250 and 350 °C. Structural characteristic of the samples are discussed using x-ray diffraction (XRD) patterns, Fourier transformation infrared (FTIR) spectroscopy and field emission scanning electron microscopy (FESEM) images. XRD patterns showed the formation of spinel structure for all the samples with a higher crystallinity for the samples prepared at the combustion temperature of 250 °C. Also, FTIR showed the formation of octahedral and tetrahedral sites in both sets of the samples. From the FESEM images the shape of ferrite particles was observed to be polygonal with a size of about 100 nm for both sets of the samples. Vibrating sample magnetometer (VSM) was used to see the magnetic characteristics of the ferrite samples and results showed that the saturation magnetization (M_s) of the ferrites prepared at 250 °C is higher than those prepared at 350 °C. We discussed the difference between the M_s of the samples according to their degrees of crystallinity and concluded that higher crystallinity results in higher M_s of the samples. Our results can be used in developing the fabrication methods of magnetic ferrite particles with controlled magnetic and microstructural properties.

Abstract ID: 376

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Synthesis, Controllable Growth and Characterizations

Keywords: Polydimethylsiloxane, Gold nanoparticles, Composite films, Plasmonic

In situ Rapid Synthesis of Gold Nanoparticles-Poly(dimethylsiloxane) Composite Films with Tunable Plasmonic Properties

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Plasmonic metal nanoparticle-polymer composite films such as gold nanoparticles (AuNPs) on poly(dimethylsiloxane) (PDMS) have shown potentials in a wide range of applications including sensors, and optoelectronic devices. In situ synthesis of AuNPs-PDMS composite films is alternatively a promising route toward large-scale manufacturing for commercialization but remains challenges due to lack of tunable plasmonic properties and requires long periods for nanoparticle growth. Herein, we develop a rapid method for synthesizing AuNPs with different optical properties on PDMS surfaces through H₂O₂ activation and the reaction can be achieved within several minutes. Silicon hydride (Si-H) groups in the curing agents can act as a reducing agent to allow the conversion of HAuCl₄ to AuNPs, which spontaneously attached on the PDMS surfaces, whereas H₂O₂ plays an important role in increasing rate of AuNP generation. Moreover, the results suggest that plasmon resonance peaks of the composite films can also be adjusted via the amount ratio between the curing agent and H₂O₂, representing their flexibility for the use in further applications. This study opens opportunities to develop advanced materials based on employing AuNP-PDMS composite.

Abstract ID: 377

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Fundamental investigations on low-dimensional nanomaterials and their functional structures properties

Keywords: defect engineering, phase engineering, 2D materials, CVD growth, optoelectronics

Defect and phase engineering in 2D materials for Optoelectronic Applications

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Defect and phase engineering in monolayer 2D materials (MoS₂ and WS₂) are providing various opportunities to tune the properties in atomic thin layer (< 1 nm). We present CVD growth for large scale development of monolayer 2D materials (MoS₂, WS₂) with ability to control the defects and phases to tune their properties. Site specific surface modulation in atomic thin layer has been achieved by nanoindentation technique to spatially tune photoluminescence. Such local control over luminescence properties has been also demonstrated by point defect clustering driven faceted void formation. Atomic resolution transmission electron microscope aids the visualization of the hexagonal atomic arrangement, point S-defects and accumulated defects that result in faceted voids with luminescence enhanced edges. Polymorphic phase formation in single domain of monolayer WS₂ and their atomic scale behavior are studied in detail for the realization of seamless phase engineered surfaces and interfaces. Depletion width of ~2.5 μm, capturing difference in work function of ~40 meV across semiconducting homojunction between coexisting phases in monolayer WS₂ has been explored. Photo-generated carriers increases in 1H phase compared to 1T phase such that ~5 times increment in photocurrent is observed across coexisting heterophase WS₂ in electron beam lithographically patterned FET device. Interestingly, formation of heterophase cancels competing thermal mismatch and lattice strains; stabilize crack free monolayer heterostructure. Further, introducing defects onto monolayer, and atomic terminations in particular fashion paves a way to enhance luminescence properties and promotes miniaturizing of nanoscale optical devices for next generation photonic and optoelectronic applications.

Abstract ID: 378

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Magnetic Materials

Keywords: Low-dimensional magnetic systems, magnonic crystals, magnetic metamaterials

A New Class of Metamaterials: 2D Ferromagnetic Nanostructures

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In recent years, the study of low-dimensional magnetic systems has become topical for its several technological applications but also for a complete understanding of the underlying physics of magnetic nanostructures. Very recently, for their challenging features, great attention has been paid to the investigation of the static and dynamical properties of magnetic nanostructures with special regard to magnonic crystals, a class of periodic magnetic systems characterized by modulated properties. As shown by several theoretical approaches, the ferromagnetic materials composing periodic magnetic systems can be described as metamaterials since they exhibit effective properties [1]. More specifically, it is possible to define an effective magnetization and an effective permeability both in a lossless and in a lossy ferromagnetic medium, an effective wavelength and an effective wave vector for collective excitations and, under some conditions, an effective diamagnetic behavior of ferromagnetic periodic systems. Moreover, the band structure of different kinds of magnonic crystals can be determined. In this study, we give an overview of the recent results obtained on the study of metamaterial and effective properties of two-dimensional ferromagnetic nanostructures. Micromagnetic simulations and simple analytical calculations applied different kinds of ferromagnetic nanostructures allow to extract the above described metamaterial properties. Some possible applications based on the effective properties for tailoring new magnetic devices are suggested.

1. R. Zivieri, Metamaterial properties of one-dimensional and two-dimensional magnonic crystals, *Solid State Physics*, 63 (2012) 151-216.

Abstract ID: 380

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Photocatalytic and electrochemical water splitting

Keywords: photoelectrochemical water splitting, cathode materials, 2D materials, plasma engineering, MoS₂

Plasma engineered 2D-MoS₂ nano flowers decorated on Reduced graphene sheets for Hydrogen Evolution

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Water splitting is one of the important and clean method to produce hydrogen with zero carbon emission. However, the hydrogen economy and successful of production of hydrogen with electrochemical method is constrained by the nature of the best electrocatalyst (platinum) used . Indeed, platinum is having the advantage of low overpotential with fast kinetics of hydrogen evolution reaction but cost and scarcity are primary factors affecting the successful commercialization of the electrochemical method. Secondly utilization of renewable energy (solar energy) with non-noble metals/ metal oxides as transition metal chalcogenides, nitrides, phosphides, nitrides, borides serve an alternative to fulfil the conditions of low cost, low overpotential with fast kinetics for HER. MoS₂ belongs to the family of two dimensional transition metal dichalcogenides ,molecular formulae MX₂ (S, Se or Te) emerged as stable and effective catalyst for photoelectrochemical hydrogen generation. MoS₂ shows exciting electrochemical activities due to the unique physical and chemical properties. In this article, 2H-MoS₂ nanosheets were mixed with the few layers of RGO with environment friendly hydrothermal method. As oxygen (O₂) plasma exposure is an effective and promising way for simultaneously engineering the planar sites of MoS₂/RGO to fabricate the high-performance HER electrocatalysts. Here, controlled plasma exposure time has been designed to explore oxygen presence in O₂ plasma modified MoS₂/RGO catalyst towards HER performance. Morphology factor assessing the catalyst active surface factor for a series of O₂ plasma samples has been synthesized and correlated to the catalytic efficiency and synergistically tune structural and electronic modulations for HER.

Abstract ID: 381**Symposium 1: Functional Biomaterials and Biosensors (FBB)****Oral Presentation**

Topics: Wound treatment

Keywords: Mg-ATP, ATP-Liposome, Rat, Zone of stasis, Burn wound healing

Saving zone of stasis in burn wounds by intracellular delivery of Adenosine triphosphate: An experimental study in rat

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In 1953 Jackson described three zones in burn wound based on the severity of destruction and blood flow alterations. The intermediate zone, encircling the central zone is the zone of stasis, get vital but with stagnant blood supply, leading to an ischemic insult. Investigations on the pathobiology of the zone of stasis revealed that irreversible tissue necrosis ensues with progression of hypoxia and ischemia in 1-48 h, resulting in total loss of this intermediate zone. This decreased blood and oxygen delivery to the wound cells results in significantly decreased cellular energy supply. Energy is needed for every phase of the wound healing process, and the decreased availability of ATP negatively impacts nearly every aspect of the healing process. Intracellular delivery of ATP into the cells of zone of stasis may bypass the need for a fully intact blood circulation and provide much needed energy to all of the energy-starved cells to facilitate burn wound healing. We believed that, by supplementing energy supply, the wound healing process may be improved. We developed specially formulated small unilamellar liposomes for intracellular Mg-ATP delivery. The aim of this study is saving the zone of stasis in burns by intracellular delivery of adenosine triphosphate which may enhance the burn wound healing. Fifty wistar rats were involved in this study. After shaving the backs, a 'comb burn' was contacted bilaterally on the dorsum of the rats 0.5 cm lateral and parallel to the midline by using a brass probe consisting of four rows (10 x 20 mm) and three interspaces (5 x 20 mm). All rats randomly separated into five equal groups. Each group treated by Normal saline, Carbomer 940, Free Mg-ATP, Liposome, ATP-Liposome separately. Dressings were changed every day. Doppler flowmetry measurements and histopathology were used for evaluation of perfusion and viability in the zone of stasis. Blood flow measurements repeated every 24 hours and skin specimens were taken at days 3 and 21 for histopathology evaluation. Our results showed that blood flow in zone of stasis increased 24 hours post-burning in experimental groups and the differences between the results obtained from the experimental and the control groups were found to be statistically significant ($P < 0.05$) after burn creation. Histopathologically, epithelial tissue in zone of stasis in rats treated by ATP-Liposomes statistically more than the control group and sebaceous glands and hair follicles remained viable in group treated by ATP-Liposomes. Our experimental study revealed that ATP-Liposomes improved tissue perfusion and decreased the area of skin necrosis in the zone of stasis in rats. Application of ATP-Liposomes in treatment of burn injury has positive effects and causes better burn wound healing in rats.

Abstract ID: 382

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Applications of low dimensional, nano and 2D materials

Keywords: MoS₂ Nanosheets, hybridized phases, photocatalytic, adsorption

Photocatalytic and Adsorption Performance of Hybrid Phases of MoS₂ Nanosheets

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MoS₂ is very attractive material and has been well studied for potential applications in various areas [1-4]. However, due to the wide variety of factors affecting the molecular and electronic structure of MoS₂, several contradicting reports about the adsorptive and photocatalytic properties of the materials have been published. In most of these reports, the effect of the actual phase of the materials on the properties was neglected. Here, different phases of MoS₂ nanosheets (1T/2H, 1T/3R and 2H) have been obtained using the hydrothermal method with different Mo:S molar ratios and different autoclave filling ratios. The obtained materials (Fig. 1) have been thoroughly characterized using Raman, UV-vis, powder XRD, SEM, TEM and XPS techniques in order to accurately identify the existing phases (and the ratio) in each material. A comparative study of the photocatalytic and adsorption efficiency of three organic dyes (MO, MB, and RhB) has been conducted to correlate the different activity of each material to the respective phase composition [5, 6]. The results indicate a much higher performance of the 1T/2H phase compared to the 2H and 3R phases. Detailed computational studies of the different phases revealed the emergence of mid-gap states upon introducing 1T sites into the 2H lattice. This leads to the improvement of the photocatalytic activity and adsorption of the 1T/2H compared to the other prepared materials.

Abstract ID: 383

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Structure Formation in Multi-Component thin films

Keywords: Nanocellulose, Atomic Layer Deposition (ALD), Superlattice structures

Superlattice Structures of Plant-sourced Nanomaterials Hybridized with Inorganic thin films for Thermoelectric Materials

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Concerns about energy security and strong dependency on fossil-sourced raw materials are heavily boosting the industry transition towards the utilization of renewable resources. Potential of plant-derived nanoscale cellulosic materials have been successfully demonstrated in diverse applications.¹ When the peculiar features of nanocellulosic materials are coupled with the numerous functionalisation opportunities achieved via e.g. hybridization, completely new application areas such as optical materials, nanoelectronics and (bio)sensors can be anticipated for these abundant biomaterial structures. This presentation shows how inherent features of cellulose, namely low thermal conductivity and high thermal stability can be exploited as a phonon blocking material in thermoelectric superlattice structures once hybridized with electrically conductive inorganic oxide layers. Superlattice structures with alternating layers of various nanocellulosic materials and ZnO showed that resistivity and thermal conductivity of such structures can be manipulated by the cellulosic thin layer nanoarchitecture. Only a submonolayer of CNF is needed to suppress the thermal conductivity of ZnO.² Inorganic multilayer structures comprising stacks of SiO₂/Al₂O₃ deposited on CNF film (individual layer thickness of 3.7 nm for SiO₂ and 2.6 nm for and Al₂O₃) efficiently blocked the diffusion of the oxygen molecules through the CNF film structure.³ Moreover, simultaneously developed low temperature ALD processes enabled the inorganic thin film depositions on thermally sensitive biomaterials.

Abstract ID: 384

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Dielectric, Ferroelectric and Piezoelectric materials

Keywords: Ferrite, BFO, CFO, Multiferroics, Magneto electric effect.

Structural, vibrational and enhanced the magnetoelectric properties of BiFeO₃-CoFe₂O₄ nanocomposites

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As one of the well-known novel compounds, multiferroic materials have attracted significant attention due to coupling between magnetic, ferroelectric, and ferroelastic orders [1]. These materials are quite important in the investigation of the magneto-electric (ME) effect that can be demonstrated by the control of polarization with applied magnetic field and vice versa. The ME effect has been utilized in various multifunctional devices such as transducers, multiple-state memories, and spintronics [2-3]. So far, among all the multiferroic materials, BiFeO (BFO) is one of the most highly investigated ME materials as BFO exhibits both ferroelectric ($T_c \sim 1103\text{K}$) and G-type antiferromagnetic ($T_N \sim 643\text{K}$) characters above room temperature [4]. But magnetoelectric coefficient of BFO is very small and its bulk magnetization value is nearly zero [5]. However, BFO still has crucial problems such as high-temperature spintronic devices and its restriction in practical applications due to higher leakage current density, low polarization, and magnetization. To overcome these drawbacks, for a composite containing a ferroelectric (FE) and a ferromagnetic (FM) material, as the constituent materials approach nanometer dimension, domain walls of both the FE and FM components are altered resulting properties distinct from their bulk counterparts.

In this work, modification of magnetoelectric properties of BFO on addition of cobalt ferrite (CoFe₂O₄, CFO) by making a nanocomposite of BFO and CFO are investigated. CFO is a ferrimagnetic material with quite high magnetic moment. Addition of CFO to BFO, in the form of a nanocomposite, is expected to enhance the magnetic as well as magnetoelectric properties. Nanocomposites consisting of BFO and CFO, with composition range of (1-x) BiFeO₃-xCoFe₂O₄, where $x = 0.10, 0.20, 0.30$ and 0.40 have been prepared by the hydrothermal method. Structural, magnetic, vibrational and magnetoelectric properties of the prepared nanocomposites have been studied in detail to understand the role of CFO in modifying magnetoelectric properties of BFO. To explore the coupling between the magnetic and ferroelectric properties at room temperature for multi ferroic (1-x) BiFeO₃-xCoFe₂O₄, ($x=0.10, 0.20, 0.30$ and 0.40) composite system, the dielectric constant measured at various frequency as a function of magnetic field will be presented in the conference.

Keywords: Ferrite, BFO, CFO, Multiferroics, Magneto electric effect.

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Abstract ID: 385

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Surface treatment and Interface control

Keywords: cellulose thin films, cellulose xanthate, photolithography, microphase separation

Cellulose Thin Film Technology - Current Status and Future Challenges

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Here, we present our latest achievements in the field of cellulose thin film technology with a strong focus how to establish patterns ranging from the nanometer to the micrometer scale. Developed technologies involve the use of lithography (e.g. photolithography, e-beam lithography), microphase separation as well as the formation of nanostructures inside the films by e.g. in situ growth of functional nanoparticles. For all the presented materials, concrete applications, as well as their potential for translation into real products are discussed. Applications include optoelectronics, solar cells, as well as photosensitive layers and antifouling surfaces. All presented films are characterized by state of the art techniques.

Abstract ID: 386

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: Microalgal biorefinery, Tri-functionalized magnetic nanocomposite, Green & smart multifunctional composite, Concomitant cell harvesting and disruption, Improved process efficiency

Design and synthesis of a green, smart and recyclable bionanocomposite for concomitant recovery and disruption of microalgal biomass

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Microalgae have recently emerged as renewable biomass feedstock to address the global challenges of sustainable food, feed and fuel production in a biorefinery model, in spite of a question mark on its viability and sustainability, mainly for significant fossil energy input and discrete sub-optimal downstream processing without recycling expensive materials required for two important engineering unit operations, cell recovery and disruption. Hence, the present study was aimed at designing, synthesizing and applying green, smart and recyclable bionanocomposite bestowed with cationic, photocatalytic and magnetic properties for concomitant harvesting and disruption of microalgal biomass with nanocomposite recovery and recycling in an integrated process chain. Accordingly, dual-functionalized chitosan-TiO₂-conjugated (CTC) nanoparticles and tri-functionalized magnetic nanocomposites (MNCs) namely, chitosan coated core-shell structures of Fe₃O₄-TiO₂, were successfully prepared and characterized. The harvesting efficiency of >98% was achieved at the optimal dosages of chitosan, CTC and MNCs of 0.11 g g⁻¹, 0.09 g g⁻¹ and 0.07 g g⁻¹ *Chlorella minutissima* biomass, respectively. As evident from the scanning electron micrographs, TiO₂ driven photocatalysis could effectively disrupt harvested wet-biomass, when exposed to UV irradiation (>320 nm) in the presence of either CTC or MNCs for 4 h, and when subjected to visible light (400-700 nm) with only MNCs for 6 h. Photocatalytic cell disruption helped recover 96-97% of the intracellular lutein and lipid, as compared to ultrasonication as control cell disruption experiment. Subsequently, the MNCs were separated from residual biomass by dilute-acid treatment, resulting in >96% detachment efficiency for reuse in the downstream process chain. The recovered MNCs could be recycled for at least five consecutive batches without incurring any significant loss of biomass recovery and disruption efficiencies.

Thursday, 22/Aug/2019 2:48pm - 3:00pm

Abstract ID: 387 / FESC-2: 5

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: Graphene, Supercapacitor, Energy Storage, Green method

Graphene Based Green Supercapacitor for Energy Storage

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Electrochemical double layer capacitors also called as supercapacitor have emerged as a superior alternative to batteries technology due to its relatively high power density and long cyclic stability. Carbon based materials such as activated carbon, porous carbon and graphene etc. have been widely exploited for high performance supercapacitor owing to its extremely high surface area and superior electrochemical stability. Synthesis of graphene based materials and composites for high performance electrode materials for electrochemical double layer capacitor by green method is something icing on the cake. Here we report synthesis of graphene based composites with gold nanoparticles by in-situ reduction with ascorbic acid and further their application as electrode material in electrochemical storage device. The composite utilized as an electrode for supercapacitor in three electrode configuration exhibits maximum specific capacitance up to 300 F/g at a scan rate of 5mV/s with a very high capacity retention of ~100% up to 500 cycle. Further details related to the synthesis device fabrication and performance measurements will be discussed during presentation.

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Thursday, 22/Aug/2019 11:39am - 11:51am

Abstract ID: 388 / FLNM-2: 4

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Fundamental investigations on low-dimensional nanomaterials and their functional structures properties

Keywords: Carbon nanotubes, Nanocomposite, Raman spectroscopy, Modeling

Encapsulation of red-light-emitting phosphors in single-walled carbon nanotubes – from experiments to models

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The filling of carbon nanotubes (CNT) with crystals, ions, and organic or inorganic molecules is of primary importance to better understand the templating role of CNTs for the self-assembly of functionalized architectures at the nanoscale level [1-5]. The present work describes the structure and vibrational properties of new hybrids of CNTs and phosphors emitting in the near-infrared spectral region (NIR). Several NIR applications of these nanocomposites can be envisioned such as infrared transmissions, CNT lasers, light harvesting for photonic devices, and fluorophore release. Red emitting molybdenum octahedral clusters have been encapsulated inside CNTs in order to tailor phosphorescent probes or to switch-on efficient photoexcitation energy transfer from the phosphor to the CNT. These nanocomposites have been characterized with high-resolution electron microscopy (HRTEM) and Raman spectroscopy which are then modelled with ab initio and semi-empirical methods combining geometry optimization and vibrational calculations. The models provide hints about how charge transfer between intercalated species and nanotube walls occurs in the hybrids. This investigation is relevant to prediction of possible structural variations and physical changes of encapsulated functional molecules or ions under strong confinement.

Abstract ID: 389

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Polymeric composites

Keywords: PVDF, KNN, Ferroelectric polymers, Hybrid materials, Lead free

Synthesis and Characterization of PVDF/KNN composites

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In the last years, ferroelectric polymers have received great attention from researchers because their use in optical and electronic devices. Among these polymers, it can be cited the polyvinylidene fluoride (PVDF) because their excellent electric properties in comparison with another ferroelectric polymers. However, these properties are lower than other ferroelectric materials, such as PZT ceramics, for example. In this sense, the hybrid materials as polymers/ceramic bring a new trend of materials. From literature, it can be found a great number of papers that report the lead-based ceramic insertion into PVDF matrix improves its properties. Although, the lead oxide evaporation of those piezoelectric ceramics during the sintering process harms the environment, leading to antilead legislation in many countries. In this way, the sodium potassium niobate (KNN) solid solution, that is a lead free ferroelectric ceramic, might be a new candidate to be used to improve the ferroelectric properties of PVDF samples. Therefore, in this work the PVDF were doped with KNN ceramic in different concentrations were synthesized and characterized. The experimental measurements revealed that PVDF/KNN composites have similar properties than other lead based composites, being a potential candidate to be used in electronic devices.

Abstract ID: 390

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Advances in the Synthesis and Characterization of low dimensional, nano and 2D materials

Keywords: Semiconductor Material, MoS₂ Nanoparticles, Laser Ablation

Colloidal Synthesis of Nano MoS₂ by Nanosecond Laser Ablation of a Bulk MoS₂ Target in an Organic Solution

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Molybdenum disulfide (MoS₂), is a semiconductor material with a layered structure and the great antifriction performance [1]. The application of MoS₂ has extended into the field of future electronic circuits requiring low stand-by power, catalysis, electrochemical intercalation, solid lubrication, optoelectronic devices, electrocatalysis, solar energy funnels, composites, tumor therapy using photothermal effects with promoting apoptosis of cancer cells, photocatalytic hydrogen evolution, lithium ion batteries, and so on [2, 3]. It is important to say that the most effective approach to reducing the friction and wear at contact interfaces is the use of lubricants mixed with MoS₂ NPs [4]. Furthermore, MoS₂ particles with nanometer-scale dimensions display a good catalytic activity, a low friction coefficient, and unique physical properties compared with their bulk material. Furthermore, they possess a large active surface area, increased adsorption capacity, excellent electrical conductivity, high reactivity, and complete resistance against oxidation in a moist air environment [5]. In this paper, MoS₂ NPs with spherical and flower-like structure were prepared by 1064 nm laser ablation (Nd:YAG, 7 ns, 10 Hz, 6000 pulse, a focal length of 20 cm) of bulk MoS₂ target at different laser fluences of 0.8, 1, 1.2, and 1.4 J/cm² in Ethylene Glycol, at room temperature. The morphology, crystal structures, chemical, and optical features of MoS₂ NPs were characterized by Ultraviolet-Visible (UV-Vis) spectroscopy, X-ray diffraction (XRD), Transmission Electron Microscopy (TEM), selected area electronic diffraction (SAED), Fourier Transform Infrared (FTIR) spectroscopy, and Raman spectroscopy. The analysis results revealed that these particles can be successfully prepared with diameters in the range of 5-130 nm and the hexagonal crystalline structure. Laser ablation technique is emerging as a simple, green alternative strategy, and reproducible way to produce a large number of attractive nanometric structures with special properties.

Abstract ID: 391**Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)****Oral Presentation**

Topics: Computational modeling and simulation of low dimensional, nano and 2D materials

Keywords: Doped Phosphorene, ambient stability, ab-initio molecular dynamics

Metadynamics Biased Ab-Initio Molecular Dynamics Studies of Doped Phosphorene for Increased Ambient Stability

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Phosphorene is an exciting material which in theory could open doorways to many different engineering applications. However, in practice it is severely limited by its degradation in ambient air conditions. Previous studies have indicated that the degradation process begins by photo-oxidation of the substrate 1, with UV light in particular a contributing factor 2. Currently, techniques for improved stability include protective layers and heat treatment, but these may not always be feasible depending on the desired application of the system. Interestingly, it was recently shown experimentally that Phosphorene flakes doped with either Sulfur or Tellurium demonstrated increased ambient stability 3,4. Motivated by these studies, we set out to investigate the reasons for this positive change by conducting state-of-the-art simulation techniques. We hypothesized that by introducing these dopants O₂ splitting can be suppressed, thereby stopping the degradation process from even starting. Using Metadynamics biased Ab-Initio Molecular Dynamics the Free Energy landscape for this reaction at finite temperature can be modelled, and we will discuss the reaction activation barriers found in each doped system. Additionally, charge analysis using a variety of modelling techniques including density of states and Bader analysis will be employed to provide additional insight into this O₂ splitting process, and to highlight the effect of dopants on the system as a whole. This work will provide a better fundamental understanding of this stabilization technique, and will shed light on the benefits of employing such dopants to Phosphorene.

Key Words: Doped Phosphorene, ambient stability, ab-initio molecular dynamics

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Abstract ID: 392**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

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

Keywords: Lithium-sulfur battery, Blue phosphorene, Density functional theory, NEB, Lithium polysulfides, Diffusion

Blue Phosphorene as a cathode in Li-S batteries

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For the Li-S battery technology to succeed, while it is important to find cathode materials which can trap lithium polysulfides (LiPS) strongly to suppress the “shuttle” effect¹, fast diffusion of lithium and LiPSs over the cathode is also crucial to prevent agglomeration. We report that recently synthesized monolayer blue phosphorene (BP) possesses these characteristics. Density functional theory calculations showed that while the adsorption energies (E_b) of various LiPSs over pristine BP are reasonably strong (from -0.86 eV to -2.45 eV), defect engineering the material by introducing single vacancies (SV) increases the binding strength significantly, with E_b in the range -1.41 eV to -4.34 eV. Molecular dynamic simulations conducted at 300 K revealed that an SV can trap Li atoms in various metastable LiPSs stronger than pristine BP. Projected density of states revealed that creation of an SV induces metallicity in the materials resulting in an increase in the adsorption strength which did not lead to any significant structural deformation. The energy barriers (EA) for the larger LiPSs over pristine BP were found to be minimal to ensure ultrafast migration, with the lowest diffusion energy barriers being 0.23 eV, 0.13 eV and 0.18 eV for Li₂S₄, Li₂S₆ and Li₂S₈, respectively. Additionally, the magnitudes of EA associated with the catalytic oxidation of Li₂S over pristine and defective BP were calculated to be less than three times smaller than graphene². These results suggest that the charging processes could be faster by orders of magnitude over BP than graphene. All these observations put together suggest that BP with a suitable combination of defects could be an excellent cathode material in Li-S batteries.

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Abstract ID: 393

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Polymeric composites

Keywords: PVDF, Neodymium, Ferroelectric Polymer, Optical Properties, Optical Fluorescence

Study of the Optical Properties of Neodymium Doped PVDF

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Polymer-based optical materials have received great attention from the researchers because of its increasing use in the optoelectronic applications, such as in polymer-based light-emitting diodes, light electrochemical cells and solar cells. Among the used polymers, the poly(vinylidene fluoride) (PVDF) can be easily processed and prepared to enhance optical properties to be used as optical switches, optical waveguides, light emitting diodes, lenses and nonlinear optical devices. Recently, studies have reported the utilization of PVDF as a hosting for rare earth ions, which enables the use in optical devices. Among them, neodymium (Nd) can be cited due to their high efficiency at room temperature. Therefore, in the present study PVDF neodymium doped samples (PVDF/Nd) it was prepared in sense to enhance the optical properties of pure PVDF. X-Ray diffraction (XRD) measurements were done to analyze the crystallinity and amorphous structural behavior of the films. From SEM measurements it was possible to see that pure PVDF films presented spherulites size well defined between 3 and 4 μm , but when Nd₂O₃ was added it is observed an increasing of spherulite size and a decreasing in porosity of doped material. FT-IR measurements were done to calculate the relative percentage between β and α phases. From UV-Vis measurements it was possible to see that the Nd addition into PVDF matrix increases the optical absorbance spectrum at UV region. Fluorescence measurements showed a widening of emission band to the red region for all concentrations of PVDF/Nd. In summary, our results demonstrate that the Nd addition improves the natural fluorescence of the PVDF samples. Therefore, the obtained results indicate that the PVDF/Nd doped has a great potential to be applied in optical and photonic area.

Abstract ID: 395

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Structural analysis and Optimization of functional composites

Keywords: Polyaniline, Hexaferrite, Electromagnetic properties

Polyaniline-barium ferrite composites: An optimization study for high efficiency microwave absorption

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With the widespread applications of wireless communication technology as well as the convenience of life, people are also facing the problem of communication security, electromagnetic radiation pollution and signal interference which even threaten their health. Therefore, it becomes very important to develop new materials with improved performance to reduce the electromagnetic harmful effects [1]. The main purpose of this research is to develop composite materials based on conducting polymers such as Polyaniline (Pani) doped with different types of acids, and barium hexaferrite (BaFe₁₂O₁₉) with or without substitution according to desired stoichiometry. In the barium hexaferrite, the substitution of Fe³⁺ is made by Al³⁺, Bi³⁺, Cr³⁺ and Mn³⁺ ions.

We succeeded to elaborate Pani/BaFe₁₂O₁₉ and Pani/BaMeFe₁₁O₁₉ (where Me = Al, Bi, Cr and Mn) composites by oxidative polymerization using different pathways: Aqueous-Based Polymerization (ABP) and Solid-Based Polymerization (SBP). The optimization of these various synthesis techniques after physicochemical (XRD, FTIR, TGA, SEM, EDX), dielectric (ϵ' , ϵ'' , σ_{dc}) and magnetic (M_r , M_s , H_c , T_c , μ' , μ'') characterizations of the samples showed that the solid route is the easiest, economical and environmentally friendly method. It is also suitable for the production of composites Pani/BaFe₁₂O₁₉ with good structural, physical and magnetic properties [2].

The obtained structures show a highly dependence of the electromagnetic properties with the doping agent nature of polyaniline and the substitution effect in hexaferrite. The incorporation of the substituted hexaferrite in the polyaniline to obtain Pani/BaMeFe₁₁O₁₉ composites reveals a variation in electromagnetic properties in the frequency range from 1 to 18 GHz. In fact, these variations are due to the formation of dipoles between the substituting ion and surrounding O²⁻ cations in the ferrite which are responsible for the ferromagnetic resonance, the magnetocrystalline anisotropy and the exchange interaction with the polymer. The composite Pani/BaFe₁₂O₁₉ shows absorption bands at the X-band that shift to the Ku-band with the substitution of iron, confirming the potential of these materials for microwave applications [3].

Abstract ID: 396**Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)****Oral Presentation**

Topics: Novel 3D functional architectures consisting of low-dimensional nanomaterials

Keywords: MXene, Fibers, Supercapacitors, 2D Nanosheets, Energy Storage, Sensing

MXene Fibers: the New Member of Functional Fibers Made From Two Dimensional Nanosheets**Joselito Razal**

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Yarn-shaped supercapacitors (YSCs) once integrated into fabrics provide promising energy storage solutions to the increasing demand of wearable and portable electronics. In such device format, however, it is a challenge to achieve outstanding electrochemical performance without compromising flexibility. Metal carbides or carbonitrides called “MXene” has presented a distinct combination of very high conductivity ($\sim 10,000 \text{ S cm}^{-1}$), volumetric capacitance ($\sim 1,500 \text{ F cm}^{-3}$), and hydrophilic properties. To date, however, MXene-based fibers or yarns that can be used for wearable applications have been relatively unexplored. Their small sheet size ($< 2 \mu\text{m}$) and weak inter-sheet interactions have made it challenging to fabricate MXene-based fibers or yarns. Here, we present strategies to achieve fibers or yarns from Ti_3C_2 MXene. Our works include high-performance yarn supercapacitors fabricated by coating MXene on conductive carbon fiber bundles. This device showed length capacitance of $\sim 132 \text{ mF cm}^{-1}$ higher than the literature reports (typically lower than 100 mF cm^{-1}) even at low mass loading of 2 mg cm^{-1} . We also used wet-spinning technique by taking advantage of the templating role of liquid crystalline (LC) graphene oxide (GO) to produce fibres with high MXene content of $\sim 88 \text{ wt. \%}$. These fibres demonstrate excellent flexibility and a high volumetric capacitance of $\sim 341 \text{ F cm}^{-3}$. We also employed biscrolling technique to scroll MXene nanosheets within carbon nanotube helical corridors. Here, the yarns are predominantly MXene containing up to $\sim 98 \text{ wt. \%}$ MXene yielding an areal capacitance as high as $\sim 3,188 \text{ mF cm}^{-2}$, which exceeds the previously recorded performance for any fiber or yarn supercapacitor electrode. The supercapacitor prototype in asymmetric configuration reached a maximum energy and power densities of $\sim 61.6 \text{ mWh cm}^{-3}$ and $\sim 5428 \text{ mW cm}^{-3}$ respectively. We show that the MXene-based fibers and yarns are useful for powering small electronic devices when knitted or woven into a textile. Our works have introduced a new class of fibers that can be excellent candidates for integration within textile-based electronics and wearable devices.

Abstract ID: 397 / Poster: 1

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Nano and Environmental catalysis

Keywords: Nanoporous MOF materials, Organic linkers, Lewis basic nitrogen sites, CO₂ Capture, Catalysis

Nanoporous Metal Organic Frameworks for CO₂ capture and Heterogeneous catalysis

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Nanoporous Metal Organic Frameworks for CO₂ capture and Heterogeneous catalysis

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Design and synthesis of nanoporous frameworks has emerged as a powerful tool in order to address the world's energy and environmental problems along with industrial applications as heterogeneous catalyst. MOFs,^{1,2} a nanoporous crystalline framework composed of metal ions or clusters coordinated with rigid organic ligands or struts to form two- or three-dimensional architectures. Owing to their special characteristics such as hybrid compositions, adjustable functionality, and diverse structure, MOFs are of pronounced interest for various applications such as separation, sensing, and catalysis.^{3,4} Rational design of basic active centers allows one to substantially improve the catalytic performance,⁵ in particular, to enhance the activity and selectivity along with CO₂ capturing ability. In this context, our research focuses on design and synthesis of metal-organic frameworks (MOFs) with Lewis basic sites (N-containing ligands) for the application of CO₂ capture and heterogeneous catalysis. In this view, we have focused on the new and novel construction of metal organic frameworks (MOFs) by using the organic linkers with carboxylate functionality and metal source based on azaindole, benzimidazole, benzoxazole and benzothiazole⁵ derivatives. The MOFs are thoroughly characterized by using a variety of techniques such as (XRD), (FT-IR), (AAS),(TGA), (SEM), (TEM) and N₂-physiosorption measurements. These MOFs represent a new synthetic era in the field of organic-inorganic hybrid materials. Their unique features, such as highly flexible molecular design, permanent porosity, and controllable pore size, and the diversity of available building blocks promise that this field, although currently in its early stages, will grow into a rich and broad area of great interest.

Schematic representation for the synthesis of MOFs

Key Words: Nanoporous MOF materials, Organic linkers, Lewis basic nitrogen sites, CO₂ Capture, Catalysis.

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Abstract ID: 398**Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)****Oral Presentation**

Topics: Photonic and optoelectronic device applications of low dimensional, nano and 2D materials

Keywords: Carbon Nanotubes, Thin Films, Electrochromic, Electro-Optical, Ionic Liquid

Designing Fast Electrochromic Devices Based on Single-Walled Carbon Nanotube Thin Films

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Improving the modulation depth and switching speed of electrochromic devices is important for expanding the field of electrochromic functional materials applications. In this study we have introduced electrochromic devices with (SC-) single-wall carbon nanotube (SWNT) films as active electrochromic layers and metallic (MT-) SWNT counter electrode layers which act as transparent conducting electrodes and ion storage layers simultaneously.[1-3] This multifunctionality leads to the requirement of balancing the films thicknesses according to their electrochemical capacitances. As a result of the balancing, a modulation depth of 20 dB and fast response time of a few milliseconds were achieved,[3] as compared to the typical response times of the electrolyte controlled cells in the range of 1-100 seconds. Such balance and vertical design with completely overlapping SWNT layers allowed optimal distribution of potential across the electrochromic cell with maximum electric field driving the ion diffusion in and out of the SC-SWNT electrochromic layer and efficiently switching the SC-SWNT layer between the bleached and colored charge state. AC impedance measurements of intrinsic capacitances of MT- and SC-SWNT layers and experimental optimization of the device components showed that the optimal ratio of MT- to SC-SWNT layers thicknesses is close to 1:2. The resulted electrochromic cell shows high coloration efficiency exceeding 1800 cm² C⁻¹ due to the bleaching mechanism which does not include reduction-oxidation processes in the electrochromic material, but only refilling of the sub-bands originated from van Hove singularities of 1D SC-SWNTs. The efficient electro-optical modulation is a result of the high porosity and high surface area of SWNT thin films which allow fast penetration of the ions and the formation of a 3D electric double layer capacitor involving the full volume (thickness) of the SWNT layer. The development of fast electrochromic systems provides an opportunity to expand the field of thin film SWNT optoelectronics into smart window applications, infrared modulators and shutters, and infrared imaging systems.

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Abstract ID: 399

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Theoretical/Modelling/Computer Simulations Of Functional Materials

Keywords: Hydrogel, FEM simulation, Stimuli-responsive

Modeling of stimuli-responsive hydrogel using FEM simulation

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Hydrogels have unique three-dimensional network structure with polymeric chains that enables to swell in water up to thermodynamic equilibrium. Stimuli-responsive hydrogels have been getting a lot of attention by virtue of its unprecedented levels of control over material properties and behaviors in response to external stimuli. Recent studies providing various types of stimuli-responsive hydrogels have mostly deal with photo-responsive, pH-responsive, temperature responsive and chemically-responsive hydrogels. Here we report how to model the responsive behavior of hydrogels by analyzing their characteristics and implementing the finite element method simulation (FEM simulation). Since each stimulus or stimuli responsive hydrogel has its own unique mechanism, it is important to measure the material properties of hydrogel such as modulus, swelling, porosity, and microstructure, analysis the mechanism to the external stimuli. Once it has been established, FEM simulation enables to predict and analysis responsive behavior based on numerical calculation. In this research, we focused on the three stimuli, which are photo, temperature and humidity. The study of FEM simulations verifies that the final shapes of the hydrogel structure are governed by intrinsic properties, such as the modulus and the swelling ratio, and extrinsic geometrical factors, including the thickness ratio of the bilayer and the shape of the structure. Especially, the various deformation shape can be achieved by simply changing its intrinsic properties. This fundamental investigation not only provides insights into the responsive behavior of microstructures but also has important implications for responsive and intelligent soft matter.

Abstract ID: 400

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Bio Plastics

Keywords: Bio-plastics, Polyhydroxybutyrate, Bacillus cereus, Oil-industry byproduct, Proteome analysis

Production of Bio-plastics Polyhydroxybutyrate by Bacillus cereus tsu1 Using Canola-based Oil Industry Byproduct

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Polyhydroxyalkanoates (PHAs) are a family of bio-based and bio-degradable plastics, which naturally found in a large number of bacteria that accumulate it as a reservoir of carbon and energy. The unique properties of PHAs derived materials like insolubility in water, biocompatibility, oxygen permeability and UV resistance have driven comprehensive studies and applications as packaging material, medical material, chiral drugs, etc. Polyhydroxybutyrate (PHB) is one of the most well studied bio-polymer in the PHAs family, the commercialization of which is limited by its high production cost as compared to that of petroleum-based one. Bacterial strain Bacillus cereus tsu1 with PHB-producing activity was isolated at Tennessee State University. PHB production efficiency of 'tsu1' when cultured on rapeseed cake aqueous extracts which are byproducts of the canola-based oil industry, were conducted, this results in 558mg of dry cell biomass and 14% PHB content. The physical properties of 'tsu1' PHB extracts were found comparable with standard PHB compound (sigma) using Xplora Raman spectrometer and Nicolet IS10 Fourier transform infrared spectroscopy.

When 'tsu1' was cultured in rapeseed cake substrate (RCS, 25g/L) for continuous 12, 24 and 48 hours and inspected intracellular PHB accumulation status by Sudan black staining. PHB accumulation was observed starting at early exponential phase, PHB degradation started after 12 hours at stationary phase, and completely vanished after 48-hour culture. Bacterial cell pellet at the three time points was collected for intracellular protein extraction followed by a TMT-labeling quantitative proteomic analysis to examine the proteome profile differences underlining this physiological change. Altogether, there were 2,952 proteins got quantified, protein abundance of PHB polymerase /PhaC is 1.5-fold higher in 12-hour sample compared to that of 48-hour sample. Repression protein /PhaR is 1.58-fold higher in 48-hour sample compared to that of 12-hour sample. The abundance of intracellular PHB depolymerase /PhaZ, and one esterase (with PHB binding site) nevertheless were found higher in the 12h sample. These results imply that the PHB product is utilized and synthesized simultaneously. Strategies for a higher PHB yield may be achieved by intracellular PHB depolymerase knockout.

Abstract ID: 401

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Electrochemical Supercapacitors

Keywords: supercapacitor, graphene, supermolecular self-assembly; N, P-codoping

Supermolecular Self-assembly Promoted Porous N,P-Codoped Reduced Graphene Oxide as a High Performance Electrode Material for Supercapacitors

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Inspired by supermolecular self-assembly strategy, nitrogen and phosphorus co-doped reduced graphene oxide (NP-rGO) material was prepared by hydrothermal treatment from the supermolecular system of melamine, phytic acid, and graphene oxide (MPA/GO). Here, MPA not only acts as a “sacrifice template” to promote the formation of uniform three-dimensional (3D) porous structure, but also as a barrier to prevent the graphene sheets from aggregation, as well as the precursor of nitrogen and phosphorus source for in-situ N,P-codoping. TEM and SEM image of P-NrGO display crumpled and loose-packed thin layer morphology with porous 3D structure. As electrode material for supercapacitor, the NP-rGO exhibits high specific capacitance (416 F g⁻¹ at 1A g⁻¹), outstanding rate capability (230 F g⁻¹ at a current density of 50 A g⁻¹), and satisfactory cycling stability (97.5% capacitance retention after 10,000 cycles), and displays notable enhanced capacitive performance comparing with the undoped reduced oxide (rGO). The NP-rGO sample was further assembled into symmetric supercapacitors, the symmetric supercapacitors possess high energy density of 15.4 Wh kg⁻¹ at high power density of 5000 W kg⁻¹. The excellent electrochemical performance is attributed to the synergistic effect of P and N doping in graphene nanosheets and the unique 3D porous structure.

Thursday, 22/Aug/2019 3:48pm - 4:00pm

Abstract ID: 402 / FTF-2: 10

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin Films in Biological and environmental Applications

Keywords: Salinity Gradient Energy, Nanocomposite Ion Exchange Membrane, Graphene Oxide, Reverse Electrodialysis, Pressure Retarded Osmosis.

Nanocomposite ion exchange membranes and free-standing graphene oxide membrane in salinity gradient energy generation

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Energy can be sustainably generated by utilizing natural salinity gradients in coastal environment. Power derived from the mixing of two different salinity solutions can be recovered as electrical energy by regulated ion and/or water transport in reverse electrodialysis (RED) and pressure retarded osmosis (PRO) systems. In RED, ion exchange membranes (IEMs) are such important components that their electrochemical properties determine energy generation efficiency. Nanocomposite ion exchange membranes have been proved to be a superb strategy to obtain highly selective, highly ionically conductive, and anti-fouling properties. By modifying conventional membrane forming material sulfonated poly(2,6-dimethyl-1,4-phenyleneoxide) (SPPO) with oxidized multi-walled carbon nanotubes (O-MWCNTs) or silica oxide in an optimal range of loading around 0.5 wt%, we have achieved a simultaneous improvement of electrochemical and anti-fouling properties of synthesized nanocomposite cation exchange membranes. To understand the mechanism of property enhancement, a modeling work combined with experimental validation has shown that not the extra ion exchange sites added to the membrane matrix, but a change of microstructure due to mixed nanomaterials that renders enhanced properties. With the addition of nanoparticles (NPs), membrane volume fraction of inter-gel phase increases while the volume fraction of sulfonated polymer segments also increases. As a result, ion exchange membranes retain more counterions, and membrane ion transport efficiency tends to increase with the incorporation of NPs. In addition, a simulation model also explains the membrane property changes upon the aggregation of NPs. Nanomaterial number concentration tends to plateau due to groups of NPs formed within the matrix. Finally, antifouling property and selectivity of IEMs can be boosted by a facile layer-by-layer deposition poly(styrenesulfonate) and poly(ethyleneimine). Capable to function in the presence of multivalent ions and natural organic matter, polyelectrolyte-modified anion exchange membrane was able to increase the maximum gross power density by up to 17% and energy conversion efficiency 3 times compared with standard AEM conversion. Other than RED, with advanced material developed for PRO, we are driving power generation more feasible. With optimized synthesis technique, freestanding graphene oxide membranes (GOMs) are made with moderate water permeability coefficient and excellent mechanical strength. Free-standing GOMs is promising in energy generation because of their ability to minimize internal concentration polarization, and therefore results in high water flux in the osmosis-driven membrane systems. Experimental work and theoretical calculation have shown that GOMs can have a power density of 24.62 W/m² at a hydraulic pressure of 6.90 bar using 3 M and 0.017 M of NaCl as a draw and a feed solution, respectively.

Abstract ID: 403

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Fundamental investigations on low-dimensional nanomaterials and their functional structures properties

Keywords: Graphene, Origami, Dewetting

Dewetting assisted selfassembly/ origami formation and folding of graphene particles

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Ever since its extraction from Graphite in 2004, the scientific and technological interest to understand the properties of Graphene, the first found 2D crystalline material, has increased many folds. All the unique properties of graphene, which make it, such an invincible material stems from its unique structure, which because of its flexibility can be morphed into different origami forms by application of external forces. The properties of controllable folding and unfolding of graphene can be useful in creating actuators. Whereas 3D stacking can improve the optical, electrical properties many folds and all this can be achieved by virtue of stress engineering of the underlying supporting material. In our present work, we try to achieve this with the help of a simple dewetting force. Up to now nanoparticle-laden polymeric films are only found to arrest dewetting. However, if such a film be cast where the concentration of the graphene particles vary throughout the lateral length, the dewetting started from the lean particle-concentration zones is seen to force the graphene particles on the extreme other zone to self-assemble. Moreover, the concentration difference of the particles also leads to Marangoni forces which lead to nano-particle walk-offs and tearing of the underlying film and folding of the graphene particles; while assembling the particles are also seen to form graphene nano-ribbons. A simple dewetting experiment, thus, has been seen to give rise to grapheme self-assemblies that range from folding, wrinkling, flake, onion-ring, blob structure formation, to twisted nano-ribbon and dendrimer formation to nanodot walk-offs leading to scratching at different zones. The dewetting assembly has been used in the present scenario as a template to understand the nature of forces essential for forming particular types of origami.

Thursday, 22/Aug/2019 2:24pm - 2:36pm

Abstract ID: 404 / FTF-2: 3

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Nanostructured and Architecturally Designed Coatings, Smart Surfaces

Keywords: Programmable Nanostructure, Quasi-Random, Photovoltaics

Programmable High-Efficiency Quasi-Random Nanostructures for Light Harvesting Devices

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Quasi-random nanostructures which are neither periodic nor fully random possess both the broadband wide-angle light trapping and customizable strong light management for the desired wavelength windows. These unique properties make them exciting photonic materials for various emerging optical and optoelectronic applications. However, the typical top-down process to fabricate order-disorder structures is expensive, time-consuming, and restricted to a limited pattern area. To overcome this challenge, in this talk, we report a programmable, easy-to-use, scalable, cost-effective, reproducible, soft nanoimprint method to fabricate quasi-random nanostructures on polymer from determinant mathematical algorithms over a large area for broadband, omnidirectional, and polarization-insensitive photon management by repurposing low-cost consumer electronic products including an optical disc and optical burner. In the optical disc technology, binary code 0 and 1 are represented by islands and pits on the optic disc. Therefore, by digitally programming the quasi-random sequence consisting of 0s and 1s, we can create the quasi-random nanostructures on the optical disc from Fibonacci and Rudin-Shapiro quasi-random sequences which then can be replicated using the nanoimprint method. To examine the omnidirectional and broadband photon management, we coat them onto various photovoltaic devices including amorphous silicon thin film solar cells, monocrystal silicon solar cells, and CIGS thin-film solar cells. Our experimental results show that the quasi-random nanostructures can significantly increase the solar cell efficiency for all three systems more than 12% over a wide range of incident angles. In particular, the Rudin-Shapiro pattern enhances the CIGS solar cell efficiency by 19.1% with over 90% external quantum efficiency in the wavelength range from 470 nm to 950 nm. Besides photovoltaics, our programmable quasi-random nanostructures with exceptional broadband and omnidirectional photon management can find important applications in broad-band LEDs and optoelectronic devices.

Abstract ID: 405

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Smart Composites

Keywords: conductive polymer, strain sensor, smart hydrogel, soft robotics

Multi-responsive Hydrogels as Flexible Strain Sensor and Actuator

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Soft sensors and actuators compliant and compatible with flexible devices become highly desirable for wearable electronics and soft robots. Conductive polymer is one kind of promising material for piezo-resistivity-based strain sensing unit due to their neuron-like electrical conductivity through the soft matrix, but a big challenge remains in combining their piezo-resistivity and good elasticity and the soft supporting substrates are usually non-responsive. “Smart” hydrogels that change their volume drastically in response to environmental changes, such as temperature, exhibit the unique capability of serving as sensorimotor like actuators. However, the low responding rate of these osmosis-driven hydrogel actuators, compared to pneumatic or hydraulic actuation, limits their applications. We have successfully integrated conductive polymers and stimuli-responsive hydrogel matrix into three-dimensional macroporous composites. These smart composite polymers present unique self-contained multi-sensing and actuating capabilities with high sensitivity and rapid responsiveness, attributed to the anisotropic 3D structure and high specific surface respectively. The presented composite can monitor both the local strain and the ambient temperature that can further induce strain and is able to be actuated by the applied heat source. This novel class of conductive multi-responsive and robust composite polymers would lead to stretchable and flexible soft sensors and actuators with high sensitivity of multiple stimuli and high actuation speed.

Abstract ID: 406

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Fundamental investigations on low-dimensional nanomaterials and their functional structures properties

Keywords: modified graphene oxide, suspensions, phosphonium ionic liquids, stability, rheology

Preparation and physico-chemical properties of suspensions of graphene oxide in solvent with ionic liquid

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Graphene oxide (GO) forms stable dilute suspensions in water but is difficult dispersing it in hydrophobic organic solvents including hydrophobic ionic liquids (ILs) to form stable suspension. Results of introductory study of surface modification of GO to achieve stable suspensions in solvents with ILs will be presented. Several hydrophobic modifiers were tested. Dispergation of GO modified with dodecylamine (GOamin) led to reasonable stable suspensions. GOamin with nitrogen content about 3% was dispersed in solvent with 70 mass% tetradecyltriethyl-phosphonium bis-(2,4,4-trimethylpentyl)phosphinate and 30 mass% dodecane or in pure IL without diluent. Suspension was homogenised in ultrasound bath (200 wat). Stability of suspension in terms of time dependence of relative height of clear solvent at top of suspension was estimated. Beginning of sedimentation was defined as time when started to form clear solution at top. Mean apparent particle size was estimated by dynamic light scattering (DLS). Temperature and shear stress dependence of suspension viscosity were measured cone and plate rheometer.

Interesting, to some extent surprising results were found. With increasing concentration of suspension its stability was increasing and particle size was decreasing. Suspensions stable more than 30 days were found at concentrations more than 0.5 mass%. Particle size at concentration 0.1 % of 700 nm decreased to about 270 nm at 2%. Smaller particles at higher concentrations are probably connected with higher frequency of particles collision. Initially was supposed that decrease in particle size was responsible for increased suspension stability. Preparing suspension with 0.1 % GOamin with smaller particles, by applying longer sonication or by its preparation by dilution of suspension with 0.5%, does not improve its stability. This suggest hypothesis on formation of structures of particles which prevent their sedimentation. Temperature dependences of suspension viscosity was correlated with Litovitz equation by good fit. Suspensions with concentration above 0.5% are non-newtonian and at concentration about 4.8% are paste like.

Influence of GO modifier and composition of the solvent on stability and properties of suspensions will be further studied. Influence of nanoparticles on affinity properties of solvents will be studied as well.

Abstract ID: 407

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Wound treatment

Keywords: Hydrogel, Pro-regenerative, Scarless Wound Healing

Pro-regenerative Hydrogel regenerates perfect skin

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Full-thickness wound healing commonly leads to non-functioning scar tissue formation in adults. Despite intensified efforts to attenuate scarring via mechanistic and, less frequently, translational studies, few innovative approaches have been developed in the pipeline. Recent progress in skin biology and biomaterial science offers the possibility to make the repair transformed into a regenerative process, which holds great potential and values in clinical wound healing management. Unlike traditional tissue-engineered dermal skin equivalents, we aim to develop instructive hydrogel scaffolds by incorporating functional groups to establish key interactions with endogenous cells in ways that unlock the body's innate regenerative powers. Based on such philosophy, we designed such novel hydrogel that allows us to create an environment that can trigger, activate different signaling pathways and instruct endogenous cells to proliferate, differentiate, and migrate to self-assemble into complete skin structures. Our in vitro screening study first identified the biodegradable hydrogel that has superior biocompatibility but causes no immune responses. We further tested it for acute cutaneous injuries, including injuries of the pre-existing scars and full-thickness skin injuries. We utilized both murine and porcine models in this study and our results demonstrate that the polysaccharide based hydrogel promoted complete skin regeneration that includes hair follicles, epithelial reticulation, and differentiated dermal, on both pre-existing scarred skin and deep full skin injuries.

Abstract ID: 408

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Polymeric composites

Keywords: Molecular Cross-linkers, Metal Oxides, Polymers

Boron-rich Clusters as Molecular Cross-linkers for Hierarchical Hybrid Materials

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Cross-linking is essential for materials to form rigid 3-dimensional (3D) structures with improved thermal/mechanical properties.¹ Despite its importance, there exist a limited number of cross-linkers that are capable of generating rigid 3D networks as well as leading to significant changes in properties. Our group has recently developed a “molecular cross-linking” approach to create hybrid metal oxides using functionalized boron-rich clusters as molecular cross-linkers.² In this work, we cross-linked polyhedral boron cluster to the network of TiO₂ using a simple solution-based method. The inherent robustness of the boron clusters enables them to withstand harsh thermal and oxidizing conditions required for the synthesis of metal oxides. The comprehensive structural characterization of this material validates a hybrid molecular boron oxide that consists of a cross-linked network of intact boron clusters within which are embedded TiO₂ nanocrystals in the anatase phase. The unique structure of the hybrid material exhibited dramatically enhanced electro- and photochemical properties than that of pristine TiO₂, evidenced by fast electron-transfer rates, low resistivity and photocatalysis under visible light conditions.

We further explored the possibility to cross-link boron-rich clusters with organic monomers to create polymeric materials. The reaction between B₁₂-based clusters and isocyanates produced a polyurethane gel, featuring highly cross-linked networks. The polymer gel displays a mesoporous architecture confirmed by Brunauer-Emmett-Teller (BET) surface area analysis and scanning electron microscopy (SEM). More importantly, the polyhedral boron-rich clusters significantly enhance the thermal stability of the cross-linked polymer, which makes this potentially utilized as flame-resistant polyurethane foams. The successful modification of the materials ranging from inorganic metal oxides to organic polymeric materials highlights the value of molecular cross-linking as a new and previously unattainable strategy to tune the properties of materials for diverse applications.

Abstract ID: 409

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biomaterials for soft tissue applications

Keywords: Conducting polymers, Functionalization, Biomimetic properties

Polymer Electronic Materials for Biomedical Applications

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With the vision of mimicking the many functions found in nature, such as stretchability, healing and sensing, the next-generation of organic electronics and bioelectronics will require electronic materials with biomimetic features. Organic electronic materials, notably conjugated polymers, offer many advantageous properties - the most valuable being versatile synthesis by molecular design, ease of chemical functionalisation and solution processability.

In this presentation, I will demonstrate that the valuable biomimetic properties can be expressed through molecular design and side chain functionalisation of conjugated polymers. I will present a simple, yet versatile, synthetic procedure that enables one to fine-tune the electrical and mechanical properties without disrupting the electronic properties of the conjugated polymer. We exemplify various biomimetic properties, including stimuli-responsiveness, bio-sensing, anti-fouling, intrinsic stretchability and self-healing, by grafting polymeric side chains that affords biomimetic properties. I will also discuss recent developments of this new class of materials and their potential uses in biomedical applications.

Abstract ID: 410

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin Film Growth & Epitaxy

Keywords: CaZrO₃, Thin film, Capacitor

Preparation and Characterization of CaZrO₃ films prepared by RF sputtering technology

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Preparation and Characterization of CaZrO₃ films prepared by RF sputtering technology

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Increasing demand for high density integration of capacitor in microelectronics industry has greatly accelerated the exploration of advanced functional dielectric films including paraelectrics and ferroelectrics with high capacitance density. The paraelectrics films, such as SiO₂, Si₃N₄, and epoxy et al, are very stable to temperature, frequency, voltage, time and film thickness, but generally show a very small dielectric constant (<10). Thus there is an urgent requirement for developing the paraelectrics films with high dielectric constant. Among these paraelectrics, CaZrO₃ is an interesting material with relatively high dielectric permittivity (25-30), low dissipation factor (<<0.01) and high stability, which have great potential in the thin film capacitor application. This paper report the preparation of high dielectric constant CaZrO₃ films prepared by RF sputtering, and the effect of the Ca content, the Zr content, substrate temperature and the Ar/O₂ ratio on the films dielectric performance were studied. This CaZrO₃ films exhibit the high dielectric constant (>20), relatively low loss tangent (<0.008) and the high stability under high voltage, wide frequency and temperature range. This work suggests that the CaZrO₃ thin would be a promising candidate for thin-film integrated capacitor applications.

Figure 1 the cross-section scanning electron microscope (SEM) photographs and Polarization-electric field (P-E) hysteresis loops of the CaZrO₃ films

Key Words: CaZrO₃, Thin film, Capacitor

Abstract ID: 411

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Diagnostic and therapeutic biomaterials

Keywords: Functional DNA, Rolling Circle Amplification, Drug Delivery, Biosensor, Hydrogel

DNA Polymer Synthesized from Rolling Circle Amplification and Its Biomedical Applications

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DNA self-assemblies from the products of rolling circle amplification (RCA) have attracted great research interests.¹⁻² The reason is that, by this technique, a high quantity of meaningful sequences equipped with either designable functions or self-assembly capabilities can be produced. The resultant DNA self-assemblies have some similarities to DNA origami, which are less sophisticated but more practical for biomedical applications. Here we report a method to automatically produce hydrogels by RCAs. In this method, the functional cross-linking sites are introduced to the polymeric DNA chains on the meantime of RCA amplifications; and the properties of the hydrogel can be tuned in a very facile way through template design.³⁻⁵ Furthermore, we developed some methods to fabricate and functionalize nanoparticles from the RCA products for biomedical applications. The resultant DNA nanoparticles show designable functionalities, low cytotoxicity, and high stability in serum.⁶⁻⁷

Abstract ID: 412

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Ferroelectric film

Keywords: Breakdown Strength, Thin film, Capacitor

Enhancement of breakdown strength of ferroelectric films by constructing an oxygen vacancies migration barrier

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Future progress and new application opportunities for all capacitive devices will rely upon the ability to develop new, more advanced dielectrics with high performance and stability under high electric fields, high temperature, wide frequency range, long duration as well as requiring the harsh environment like high humidity. Relying on the rapid development of ferroelectric hetero-structure films and interface engineering, thin-film integrated capacitors with high capacitance density would be realized to meet the increasing requirement of developing miniaturized and integrated capacitor devices through the preparation of multi-interface multilayer ferroelectric hetero-structure films. Except for the obviously enhanced dielectric performance, insulation resistance is a very important parameter of the performance for the capacitor working in a high voltage range since the loss of insulation resistance would directly lead to the possible failure of the entire electronic system. However, insulation resistance and the loss of insulation resistance as a function of time and high voltage was reported only by a few studies in the ferroelectric hetero-structure films. According to the studies of degradation problems of ferroelectric devices, oxygen vacancy migration near the metal cathode is a most important cause for the degradation of performance reliability and lifetime. Even the doping method could be an effective method to suppress the oxygen vacancy density in a ferroelectric materials, there still exists a trade-off between dielectric performance and insulation resistance. However, the success of hetero-structure in the film fields provide us the new idea to solve the oxygen vacancy migration by constructing a hetero-structures to control the oxygen vacancies migration. In the present work, the insulation resistance of (Ba,Sr)TiO₃ (BST) ferroelectric thin film was effectively improved by inserting a very ultra-thin SrTiO₃ (STO) layer between the ferroelectric thin film and the electrode. This result indicates that construction of hetero-structures to control the oxygen vacancies migration would be a viable approach to improve the insulation resistance of ferroelectric films without the cost of dielectric performance.

Figure 1 I vs V and Ln(I) vs ln(V) curves for the Pt/LNO/BST/Au and Pt/LNO/BST/STO/Au films

Abstract ID: 413

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Solar Cells

Keywords: Carbon Nanotubes, Solar Cell, 3D, Fiber-shaped Electrode

Carbon Nanotube Yarn Based Three Dimensional Photovoltaic Microwires

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Fiber shaped solar cells received increasing attention in the past few years due to the flexibility, lightweight, and wearability. Fiber shaped solar cells that are not metallic have potential applications in military and functional textile. Recently, carbon nanotube yarns have attracted a great deal of interest in photovoltaic devices as potential electrodes materials due to their excellent electrocatalytic activity, high mechanical integrity, and lower electrical resistance. In this work, we utilized to carbon nanotube yarn as both working and counter electrode to developed three dimensional dye-sensitized and perovskite solar cells. The functionalization of the carbon nanotube yarn with TiO₂ offer several advantages and the TiCl₄ annealing of the TiO₂ layer results in a uniform oxide morphology. The three-dimensional dye-sensitized structure utilized TiO₂ as photo-electrode, CdS/CdSe QD as photosensitizer. Methylammonium lead iodide (CH₃NH₃PbI₃) worked as the light absorbing layer and TiO₂, and spiro-OMeTAD worked as the electron and hole transporting materials respectively in perovskite solar cell. The photovoltaic cells were fabricated through a simple and energy saving process. The all-solid-state three-dimensional dye-sensitized solar cells exhibited a maximum photon to current conversion efficiency ($\eta_{AM1.5}$) of 7.6%, and the perovskite solar cells exhibited 0.631% power conversion efficiency. The fabrication strategy of carbon nanotube yarn based photovoltaic cells could open the doors towards efficient flexible solar cells for large-scale applications and shows promising prospects to be integrated into portable and wearable textile electronics.

Abstract ID: 414

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Polymeric composites

Keywords: Nanoparticle, Polymer Brush, Membrane

Functional nanoporous materials from assembly of polymer-brush nanoparticles

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We developed a new approach for the preparation of functional membranes using polymer brush nanoparticles (“hairy” nanoparticles, HNPs). We design these membranes with molecular and ionic transport controlled by the pore size, polymer structure and environmental conditions. Our approach provides novel types of functional membrane materials with applications in separations, fuel cells and lithium batteries.

In this talk, I will describe the preparation and properties of several responsive membranes, including gated silica membranes pore-filled with temperature-responsive poly(N-isopropylacrylamide) brushes and pH-responsive poly(2-dimethylaminoethyl methacrylate) brushes, and ultrafiltration membranes reversibly assembled from HNPs carrying poly(2-hydroxyethyl methacrylate) brushes. I will also talk about proton-conducting poly(styrenesulfonic acid)- and poly(3-sulfopropylmethacrylate)-HNP membranes designed for applications in fuel cells. I will then focus on our latest results in developing charged responsive nanoporous membranes assembled using HNPs carrying polyelectrolyte brushes. I will describe the different mechanisms of transport selectivity in charged HNP membranes as well as polymer-polymer interactions in these materials that lead to their formation and stability. Finally, I will discuss our current work towards the preparation of pH- and temperature-gated HNP membranes.

Abstract ID: 415

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Solar Cells

Keywords: Chlorination, polymer solar cell, stability

Chlorination: A Facile Method for Efficient Solar Conversion

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With the development of material engineering, interface modification, and advanced device processing in past decades, the power conversion efficiency (PCE) of the state-of-the-art PSCs has already exceeded 13% at present.¹ Especially, the benzothiadiazole-T4 families of polymers, such as PffBT4T-2OD, have attracted tremendous research interest in academic communities since they can be processed into highly efficient fullerene/polymer solar cells with power conversions up to 10%. Herein, we designed and synthesized a chlorinated polymer donor, PBT4T-Cl, in which a chlorine atom had been introduced at the middle thiophene unit to fine tune the energy level of the final polymers.² Compared with its non-chlorinated analog, the PBT4T-Cl-based devices exhibited clear increases in open-circuit voltage and fill factor, achieving PCEs up to 11.18%, which is the highest PCE of a chlorine-based PSC reported to date. GIWAXS analysis illustrated the strong crystallinity from the blend films, AFM and TEM measurements both revealed an optimized morphology of the spin-coated PBT4T-Cl blend films, all of which supported that chlorine substitution could promote the performance of PSCs. More importantly, the PBT4T-Cl-based devices showed superior stability, with a PCE of 8.16% after 50 days device storage, while the non-Cl-analog-based devices remained at only 5.36% in a parallel experiment. Through this research, the chlorination of low band gap polymers provides new insight into designing π -conjugated polymer semiconductors and realizing further enhancement of polymer solar cell efficiency as well as stability

Abstract ID: 416

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Fuel Cells

Keywords: Nanoparticle, Polymer Brush, Membrane, Fuel Cell, Battery

Fuel Cell and Lithium Battery Membranes from the Assembly of “Hairy” Nanoparticles

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This talk will describe a novel approach for the preparation of proton and lithium conducting membranes using “hairy” nanoparticles (HNPs). HNPs are prepared by surface-initiated atom transfer radical polymerization (SI-ATRP). In both cases, ion-conducting channels are formed in the interstitial spaces between the nanoparticles.

Proton conducting membranes were prepared using silica nanoparticles (SNPs) surface-grafted with sulfonated polymer brushes, poly(3-sulfopropylmethacrylate), pSPM, and poly(4-styrenesulfonic acid), pSSA. Proton conducting pore-filled membranes were prepared from nanoporous colloidal crystals first assembled from unmodified SNPs, followed by filling the pores with pSPM or pSSA brushes. A sigmoidal dependence of the proton conductivity on the amount of sulfonic acid groups was found for pSPM pore-filled membranes.

Lithium conducting membranes were prepared using SNPs surface-grafted with PEO-containing polymer brushes, poly(ethylene glycol) monomethyl ether methacrylate and with poly(ethyl methacrylate). These materials showed high ionic conductivity and unusual conductivity temperature dependence.

Abstract ID: 417

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Intelligent biomaterials

Keywords: biomolecular memristor, alamethicin, memristor, ion channel, biomolecular memcapacitor, electrostriction, biomembrane, neuromorphic computing, lipid bilayer

Electrostriction, capacitive susceptibility, and neuromorphic computing in biomembranes

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Up to now, neuromorphic elements have been predominantly solid-state devices which simulate the resistive and capacitive behaviors needed for neural networks and brain-inspired computing, but in non-brain-like ways. We are integrating lipid and polymer bilayer membranes with micro- and nanofabrication to develop fundamentally new types of neuromorphic elements that have the composition (biomolecules), structure (biomembranes), and switching mechanism (voltage-sensitive ion channels) of real biological synapses, and operate at lower power than the current state-of-the-art. Our devices consist of insulating, nm-thick lipid or polymer-based bilayer membranes that assemble at the interfaces of two or more aqueous droplets in oil, and that have demonstrated both memristive and memcapacitive behaviors, including memory resistance and capacitance, synaptic functions such as paired-pulse facilitation and depression, spike rate dependent plasticity, voltage-dependent inactivation and recovery, and charging hysteresis. These behaviors are linked to electrostriction, an electromechanical phenomenon that encompasses both electrowetting and electrocompression in the membrane, which are changes in membrane area and thickness due to charging in the presence of electric fields. Electrostriction results in a voltage-dependent capacitive susceptibility that replaces the more familiar concept of static capacitance, which, up to now, has dominated electrophysiological descriptions and characterizations of biomembranes. In this picture, biomembranes are not just equivalent RC circuits dependent only on ionic currents controlled by the conductance (resistance) of ion channels. Large capacitive currents from small voltage inputs can be generated as well for the development of neuromorphic computing elements exhibiting both short-term and long-term synaptic plasticity.

Thursday, 22/Aug/2019 3:12pm - 3:24pm

Abstract ID: 418 / FTF-2: 7

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Ferroelectric film

Keywords: Ferroelectricity, HfO₂, Thin film, Phase transformation, Memory

Appearance and Disappearance of Ferroelectric Phase in Crystalline HfO₂ Thin Films Induced by Annealing Procedure

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Amorphous phase HfO₂ thin films are nowadays utilized as the high-k gate dielectric film of advanced field-effect transistors in large-scale integrated circuits (LSI). Once HfO₂ films are crystallized, they present interesting dielectric properties depending on their crystal phases. HfO₂ crystals are metamorphic and have cubic, tetragonal, orthorhombic, and monoclinic structures. Among the multiphase of HfO₂ crystals the orthorhombic crystal phase show ferroelectricity [1]. The effective ways for the formation of orthorhombic phase are doping metals into HfO₂ films [2] and preparing Hf-Zr-O compounds [3, 4]. Those dopant concentrations and Hf/Zr compositions are the key to enhance the ferroelectric property of the film. The ferroelectric thin films are promising for the development of memory devices on LSI.

We recently found that HfO₂ crystal phase evolutions, from tetragonal to orthorhombic then monoclinic, occur with annealing temperature and time. Crystal phases are controlled not only by the chemical composition, but also by the annealing procedure. The ferroelectric property appears at an optimal annealing temperature, but disappears when the annealing time is too long. This behavior implies that the phase transformation kinetics have a crucial role for the engineering of dielectric properties of HfO₂ thin films.

Abstract ID: 419

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin Films in Biological and environmental Applications

Keywords: Freestanding Graphene Oxide Membrane, Salinity Gradient Power, Waste Heat, Pressure Retarded Osmosis, Osmotic Heat Engine

A freestanding graphene oxide membrane for harvesting salinity gradient power and recovering waste heat

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Graphene oxide laminate membranes have been extensively studied for applications such as energy generation and storage, gas separation, and water purification. In this work, we show that synthesized freestanding graphene oxide membranes (GOMs) via a vacuum-assisted filtration method can be a great potential candidate for applications in pressure-retarded osmosis (PRO) for salinity gradient power (SGP) harvesting and osmotic heat engine (OHE) for waste heat recovering. Our synthesized freestanding GOMs have moderate water permeability coefficient and excellent mechanical strength. Due to their ability to minimize internal concentration polarization (ICP) in osmotic systems, the freestanding GOMs can achieve high trans-membrane water flux, especially when the concentrated draw solution concentration is high. Thus, the freestanding GOMs can exhibit superior transport properties than their polymeric counterpart in the osmotic processes. The GOMs can have high peak power density in the PRO system: a peak power density of 103.7 W/m² can be obtained using hypersaline brine (3 M of NaCl) and river water (0.017 M of NaCl) as a draw and a feed solution, respectively. In addition, a power density can be as high as 20.0 W/m² (with a hydraulic pressure of 6.90 bar) when using a 2 M ammonium bicarbonate solution in the OHE system for waste heat recovering. The results indicate that the freestanding GOMs can be applied in the osmotic systems for energy conversion and harvesting. This study provides a new way of designing membranes for energy harvesting in the osmotic-driven systems such as PRO and OHE.

Abstract ID: 420

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Photocatalysis

Keywords: tungsten trioxide; hydrothermal method; additives; photocatalysis

Hydrothermal synthesis of WO₃ nanostructures and their visible-light driven photocatalytic properties

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The tungsten trioxide (WO₃) nanoparticlesnanorod was weresuccessfully synthesized through a simple hydrothermal method, with sodium tungstate and hydrochloric acid as the main raw materials. X-ray diffraction (XRD), scanning electron microscopy (SEM), Raman spectroscopic, X-ray photoelectron spectroscopy (XPS) and UV-Vis spectroscopy were utilizedused to characterize the theirstructures, the morphologies morphology and the optical properties of the as-prepared samples. This study aimed in the effects investigation of different additives on the morphology of WO₃ nanostructures and their photocatalytic ability under visible light.the degradation feasibility of Methylene blue through the novel photocatalysts application, powered by visible light. The effect of inorganic ions from alkali metal salts on the microstructure of WO₃ nanostructures and the mechanism of their visible-light driven photocatalytic properties were explored.

Abstract ID: 421

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Bioengineering

Keywords: Graphene quantum dots, BSA, protein.

Protein Quantum Dots (ProQDs): Biofriendly, Bioactive and White Light Emitting Conductive Protein Hydrogel

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A new facile synthesis of biofriendly, white emitting, multifunctional, water-soluble, metal free, non-toxic, high photostable, bio-active and conductive protein quantum dots (ProQDs), reported here. This advanced functional nanoparticles, consisting of cross-linked bovine serum albumin (BSA) with functionalized graphene quantum dots. The combination of blue, green and red QDs are crosslinking with BSA then form the white emitting hydrogels, which are biodegradable and PH sensing. This synthesized ProQDs characterized and supported by TEM, SEM, confocal laser microscopy, XRD, XPS, CD, FT-IR, DLS, Raman, UV-Visible and photoluminescence spectroscopy and gel electrophoresis. Due to this reproducible and robust surface-functionality and unique optical properties of ProQDs has led to promising applications in bioimaging, cellular biology and drug delivery studies. Furthermore, as prepared conductive ProQDs, can be used as a bio-supercapacitor, bio-sensing and bio-solar cell applications.

Abstract ID: 422

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Bioengineering

Keywords: Graphene, scaffold, stem cell, functional neuron

Polymer-Graphene Nanocomposite Scaffold for the Differentiation of Mesenchymal Stem Cell to Functional Neuron

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Nerve cells are specialized type of cells that neither divide nor make copies of themselves post birth. Injuries or damage to neuronal cells might incapacitate normal body functions. Hence, there is a need for functional neurons or scaffolds that can enable neuronal differentiation to treat such injuries. This work aims at developing nanofiber PCL scaffolds with graphene nano-inclusions to differentiate mesenchymal stem cells (MSCs) to functional neurons. Graphene, owing to its excellent electrical and mechanical properties provides the desired microenvironment with appropriate topological and electrical cues, for proliferation and differentiation of (MSCs) into neurons. PCL polymer solution with dispersed graphene was electrospun. Scaffolds with specific concentration of PCL by weight and varied load of graphene as filler in the polymer matrices were prepared. Physical characterization of scaffold was performed by measuring fiber diameter, thickness, mechanical strength, FTIR and contact angle. For biological studies, sterile scaffolds were seeded with human Bone Marrow derived MSCs (hBM-MSCs) and incubated in neuronal induction medium. Cell viability, cell proliferation, Cell morphology, neuronal differentiation markers was examined. Microstructure of nanofiber scaffolds as observed by SEM, images were highly porous mimicking the extracellular matrix of native tissue. Live & dead staining and proliferation data showed that all the different scaffold compositions were biocompatible and support cell attachment and proliferation. In comparison with 15% PCL with varying graphene conc. (0.01% and 0.05%), in vitro studies revealed that 15% PCL +G0.05% exhibited the most optimal hMSCs attachment and subsequent differentiation into neurons. Cell differentiation over PCL 15%+G0.05% scaffolds also revealed best neuronal morphology, neuronal specific gene and protein expression and neuron alignments amongst all groups tested. This study indicates the role of graphene nanocomposite scaffold in the enhanced differentiation of MSCs in neurons. Presence of graphene in the scaffolds not only improved MSC adhesion, better neuronal morphology but also upregulated the number of differentiated neurons. Thus, we envisaged that graphene based nanofiber scaffold can serve as a potential graft for developing future therapies for regeneration of degenerated neuronal cells.

Abstract ID: 423

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Composite structural materials

Keywords: Carbon Nanomaterial, Rare Earth, Composite, Interface/Interphase, Mechanical property

Rare Earth Modified Carbon Nanotube-Carbon Fiber Multi-scale Reinforced Polymer Composite

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Based on the physicochemical properties determined by the unique atomic structure of rare earths and the surface structure characteristics of carbon nanomaterials (carbon nanotubes, graphene), this study selects rare earth element mainly lanthanide trihalides (LnH_3) with high coordination number (CN) to modify the surface structure of carbon nanomaterials. Modified carbon nanomaterial can form covalent dative bond with carbon fiber to improve the surface wettability, dispersion rate and polymer-carbon interfacial adhesion. With the increased surface activity of the carbon fibers, high interfacial strength can be obtained, therefore, high-performance carbon fiber reinforced polymer (CFRP) materials can be achieved. Owing to the high CN of LnH_3 , modified carbon fiber surface structure will not only provide enhanced interfacial bonding between carbon fillers and polymer matrix (Epoxy resin, polycarbonate, polyimide and polytetrafluoroethylene), but also improved stress transfer due to mechanical interlocking. Mechanical test (tensile, Charpy impact, flexural) was carried out to study the influence of rare earth to the mechanical strength of CFRP. Atomic force microscope (AFM) and Scanning Electron Microscopy (SEM) was utilized to characterize the surface structure of carbon composite and investigate the influences of fiber/matrix ratio, fiber dimension, state and distribution of lanthanide on carbon nano-fillers at the interfacial layer. X-ray Photoelectron Spectroscopy (XPS) and Fourier Transform infrared Spectroscopy (FTIR) was employed to identify the functional groups, and carbon fiber surface composition. In addition, the influences of multi-scale strengthening mechanism of carbon fiber and its interfacial layer on the mechanical and tribological properties of CFRP was analyzed. Finally, the strengthening mechanism of rare earth modified carbon fibers in the composite material was concluded. The accomplishment of this study suggests a new technique in multi-scale strengthening of CFRP to realize performance control of CFRP.

Abstract ID: 424

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Micro/Nano-electronics and MEMS

Keywords: TFET, Nano-device, Tunneling, Low Power Applications

Line Tunneling Based TFET for Low Power and High Speed Switching Applications with Improved Linearity

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In this paper, an optimally designed line tunneling based dual metal gate tunnel FET is presented. A silicon epitaxial layer is sandwiched between the source and gate such that dominant carrier tunneling of the device remains in-line with the gate electric field. This suppressed the lateral tunneling path which was responsible for the depreciation of the subthreshold slope, thus resulting in a super-steep subthreshold slope. The design parameters are chosen such that the device fulfills the high-performance ON-state current of 1.2 mA, low standby power OFF-state current nearly 3.53 fA and Subthreshold Swing (SS) of 37mV/decade. Moreover, the proposed TFET follows the International Technology Roadmap for Semiconductors (ITRS) roadmap for low standby power switch performance as ON current/OFF current ratio $\left[\frac{I_{on}}{I_{off}} \right]$ of the order of $\left[10 \right]^{11}$. The reduced SS makes way for the device to find application in high switching speed devices. Further from the previous researches, it is noticed that accurate evaluation of linearity of the device is of utmost requirement. So, the linearity of the proposed device is investigated in terms of VIP3, IMD3, IIP3 and 1-dB compression point. Also, the impact of temperature variation on linearity of the device is studied to better understand the stability against temperature variations.

Abstract ID: 425**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Invited Talk**

Topics: Solar Cells

Keywords: solar cells, defects, metastability and reliability issues

A Unified 2D Solver for Modeling Carrier and Defect Transport in CdTe Solar Cells

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There are many tools and software packages like AFORS-HET, SCAPS-1D, AMPS-1D, PC1D, Silvaco TCAD, Sentaurus etc., which are available freely or commercially for modeling solar cells. They offer modeling which is very useful when one knows the effective lifetimes of the materials in question. As the solar cell ages the performance is affected. This can be microscopically explained through the transport of different defects present in the solar cell. The transport of defects can also cause metastability in solar cells. In our previous work we explained the metastable behavior of CdTe solar cells by studying the Cu related defect transport along with the carrier transport [1,2,3].

In this work, we present a novel Unified Solver for studying carrier and defect transport on an equal footing. The drift-diffusion equations for defects require the diffusion constants and activation energies of the defect to be known, and the defect chemical reaction require reaction rate constants to be known. These parameters are calculated using Density Functional Theory (DFT) [4].

Since the main goal of our research work is to study short time metastability and long-time reliability concerns of CdTe-photovoltaics, special attention has been placed in the design of the solver to be able to produce results ranging from ns to hours/days/years. The solver gives us possibilities to explicitly account for all transient effects with free carriers (simulation of time resolved photoluminescence) and defects (simulation of performance instabilities, IV hysteresis etc.). Various generation-recombination processes can be represented as additional defect chemical reactions. Moreover, the Unified Solver supports accurate treatment of interfaces and grain boundaries that are crucial for the explanation of the operation of CdTe and other chalcogenide PV technologies.

The Unified Solver is applied to a constant temperature 2D simulation of chlorine diffusion annealing in a cadmium telluride (CdTe) system under insulating boundary conditions (isolated system). The time evolution of chlorine substitutional defect (Cl_A⁺) is presented. The Unified Solver also allows one to emulate process temperature profiles, which will also be presented at the conference.

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Abstract ID: 426**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Sodium Ion Batteries

Keywords: Polymers of Intrinsic Microporosity, Sodium-Sulfur Battery, carbon-sulfur composites

Carbon-sulfur composites derived from polymers of intrinsic microporosity for RT Na-S rechargeable batteries

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The growing demands of next-generation ever-increasing energy storage systems with high-energy necessitate advances in various next-generation batteries such as lithium sulfur^{1, 2} and sodium sulfur batteries^{3, 4}. Among these advanced battery systems, room temperature sodium sulfur (Na-S) battery have attracted attentions because the battery systems is based on abundant, low cost and environmentally benign elements, sodium and sulfur.^{5, 6} Aside from these benefits, both sodium (Na) and sulfur (S) possesses a high theoretical specific capacity of 1166 mA h g⁻¹ and 1675 mA h g⁻¹, respectively.⁷ Especially, room Temperature Na-S (RT Na-S) batteries have been considered as a reasonable option due to safety problems and low operating cost.⁸ However, low electrical conductivity of sulfur and polysulfide dissolution still exist so as to fully exploit the potential of these Na-S batteries.^{1, 6} Especially, the soluble long chain sodium polysulfide (Na₂S_x, 4 < x ≤ 8) can cause problematic shuttle phenomenon between the anode and cathode, reacting with Na metal anode, resulting in low Coulombic efficiency during discharge and charge cycling.⁹ In this work, Carbon-sulfur composites derived from polymers of intrinsic microporosity was investigated as a cathode material for RT Na-S batteries to suppress the problematic shuttle effect. For the preparation of the sulfur-carbon material, polymers of intrinsic microporosity (PIM-1) was employed as the carbon precursor, which polymers have the advantages of ultra-micropores. Benefiting from both ultra-micropores (~0.5 nm) and covalent bond of the resulted sulfur-carbon composites via facile heat treatment, the reoxidation to high order soluble sodium polysulfide (Na₂S_x, 4 ≤ x ≤ 8) was fundamentally inhibited. The strategy lead to the long cycling stability for 100 cycles with capacity of 400 mA h gs⁻¹ and Coulombic efficiency of approximately 100% was exhibited. This study may provide a new strategy for the design of cathode materials with long-term cycling stability in RT Na-S batteries.

Key words : Polymers of Intrinsic Microporosity, Sodium-Sulfur Battery, carbon-sulfur composites

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Abstract ID: 427

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Protective Coatings in Severe Environments

Keywords: Polyurethane, self polishing, Antifouling

Self Polishing Properties of Antifouling Polyurethane Coatings

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Antifouling paints are being used widely to prevent the adhesion of marine organisms on immersed surfaces. Unfortunately most of the commercial paints contain toxic biocides. The development of a new type of environmentally friendly/less toxic antifouling paint which has excellent antifouling performance and no persistence in the marine ecology is highly necessary. In this study, a series of self polishing polyurethane (PU) is considered to be applied as a new antifouling paint matrix. PU resins were synthesized by using different diisocyanates and polyols. Different carboxyl salts were used in PU resin. The self-polishing property with different types of monomers also measured in artificial salt water.

Abstract ID: 428

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Photocatalysis

Keywords: TiO₂, SiO₂, Photocatalyst, organic pollutant, the TiO₂/SiO₂ mixture

On-site photolysis effect of paper coated by a composite of titanium dioxide and rice husk silica with an enhanced photocatalyst

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Titanium dioxide (TiO₂) has many properties such as chemical stability and high catalytic activity. With a large oxidizing power, TiO₂ is used as a photocatalyst, Dye-Sensitized Solar Cell (DSSC), semi-conductor. Moreover, Silica is applied for filler, release carrier, insulation for catalysts having porosity property. Silica nanoparticles, in this study, were synthesized from rice husk obtained after rice threshing, which is economical compared and eco-friendly with the conventional method using silica precursor. This study is focused on confirmation of photolysis performance conveniently in on-site with paper type coated by the mixture of TiO₂ and RH-SiO₂ (TiO₂/RH-SiO₂) with its high surface area and photocatalytic activity.

TiO₂ commonly have three type of crystallinity such as anatase, rutile, and brookite, which these phases make an impact on the photocatalytic effect. TiO₂ Calcined at 200 °C (T200) was amorphous, TiO₂ Calcined at 500 °C (T500) was pure anatase and TiO₂ Calcined at 700, 900 °C (T700, T900) had both rutile and brookite. As a result, T200/RH-SiO₂ was observed higher photolysis performance in aqueous condition comparing with T200, having the high specific surface area of RH-SiO₂. Therefore T200/RH-SiO₂ was selected to spread to paper and the samples conducted to confirm the photolysis effect in on-site according to decompose the dye on the paper enough to check with bare-eye. With these results, T200/RH-SiO₂ have a potential to apply to decompose for the organic pollutant coated on the surface of object no matter how big it is.

Abstract ID: 429

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Realization and application of nanodevices electronics, optoelectronics, photonics, energy harvesting, biological sensing, composite, and so forth

Keywords: Reduced Graphene Oxide, Field effect transistor, Solution-gated FET, Amyloid-beta Detection, Alzheimer's Disease

Reduced Graphene Oxide (rGO) Based Solution-Gated Field Effect Transistor for Biosensing Platform

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Graphene, the archetypal two-dimensional material, has exceptional physical, chemical, mechanical, thermal and optical properties which has attracted great interest for applications in various sensor. Especially, reduced graphene oxide (rGO) has significant benefits as graphene-based biosensor because of its ease of synthesis, low noise level in solution, high portion of chemically active sites and good biocompatibility [1] [2]. Of the various approaches of rGO-based biosensor, rGO based field-effect transistor (rGO-FET) offers excellent advantages for label free, high sensitivity and selectivity. Especially, rGO-based solution-gated FET (rGO-SGFET) has a high potential as a biosensor, owing to the possibility of being operated in aqueous solution applying small voltages and fundamental amplification properties [3].

In this study, we fabricated a reduced graphene oxide-based solution gated field effect transistor (rGO-SGFET) and evaluating its feasibility as a biological sensory platform. rGO patterns were formed via MEMS techniques—spin coating and dry-etching technique—which optimized to possess high uniformity and mass productivity. The patterns were utilized as both the active channel and biological interface of this device. A gate voltage was applied directly through the buffer solution at a low bias range ($\sim \pm 1.0$ V), and the rGO-SGFET showed typical ambipolar transfer characteristics with a charge neutrality point (the Dirac point, V_{Dirac}). A compatibility of the rGO-SGFET as a biosensor was assessed by observing the Dirac point shift (ΔV_{Dirac}) according to a concentration of amyloid beta ($A\beta$), which is representative hallmarker of Alzheimer's disease (AD). To analyze the $A\beta$, anti-amyloid beta antibody (6E10) was immobilized on the surface of the rGO-SGFET. First, the changes of ΔV_{Dirac} for $A\beta$, which ranges from 100 fg/mL to 10 ng/mL in a PBS buffer solution (pH 7.4), were analyzed. Approximately 20 mV/dec of ΔV_{Dirac} was linearly shifted with the concentration of $A\beta$ on a logarithmic scale, owing to a lower isoelectric point of $A\beta$ (approximately 5.5) than the pH value of the buffer solution. Moreover, we performed quantitative analysis the $A\beta$ spiked in two types of bio-fluid, artificial cerebrospinal fluid (aCSF) and human plasma. As a results, ΔV_{Dirac} was also linearly shifted in the $A\beta$, which ranges from 1pg/mL to 10ng/mL, and this dynamic range was similar with the value observed in PBS buffer.

Our results demonstrate that rGO-SGFET exhibit reliable sensing performance in bio-fluid. Consequently, the results imply that rGO-SGFET might be a promising candidate in the biosensor for diagnosis of AD.

Abstract ID: 430

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Organic and polymer film

Keywords: Covalent organic frameworks; membrane separation

Fabrication of Freestanding and Nanoperforated Polymer-COF Membranes with Remarkable Mechanical Properties

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Membrane separation has attracted continuous interests due to its advantages such as easy-operation, low-cost, and energy-efficiency. Covalent organic frameworks (COFs) with ordered structure, tunable pore channels and high porosity have emerged as promising materials for membrane separation application. However, the weak mechanical properties and significant defects of COF membranes fabricated via current technologies hindered their further applications. Herein, we first utilized linear polymers as building blocks to fabricate a series of polymer-covalent-organic-frameworks (polyCOFs), that can easily form highly stable, defect-free and freestanding membranes via room-temperature interfacial polymerization. Varying the synthesis conditions, we can adjust the crystallinity, porosity, mechanical properties and thickness of polyCOF membranes. Benefitting from both the advantages of linear polymers and COFs, polyCOF membranes showed much better mechanical properties than pristine COFs, and can efficiently and selectively separate organic contaminants such as dyes from water. Our discovery paves a new way for fabrication of freestanding polymeric membranes and broadens the highly-valued applications of functional COFs.

Abstract ID: 431**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Electrochemical Supercapacitors

Keywords: Hierarchical carbons, Supercapacitor, Polymers of Intrinsic Microporosity

A Hierarchically Structured Carbon Electrodes Based on Intrinsically Microporous Polymer (PIM-1) Matrix for supercapacitor

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Due to the growing demand of next-generation applications with high power and energy density, there have been growing interest in energy storage and conversion systems.^{1, 2} Among various energy storage systems from supercapacitors to batteries, electrochemical capacitors are well-known for electrochemical energy-storage devices with higher power density than batteries and higher energy density than conventional capacitors, which is placed between batteries and conventional capacitors. In the preparation of electrical double-Layer capacitor (EDLCs), various attempts have been carried out on the development of porous carbon electrodes with good electrical conductivity and high surface area and their pore characteristics such as pore size and pore size distribution (PSD) because the systems are based on carbon materials and the properties of the carbons have an important impact on electrochemical performance.^{3, 4} Especially, significant efforts has been devoted to develop hierarchically porous carbons, which enhance the overall kinetics of electrolytic reactions by providing efficient ion and electron transport pathways and facilitates electrolyte infiltration into the electrode during charging/discharging.⁵ Herein, we introduce facile method for the preparation of hierarchically structured porous carbon electrodes. For the realization of the carbon material with hierarchical pore structure, polymers of intrinsic microporosity (PIM-1) were used as microporous polymeric matrix. To introduce the meso and macroporous structure, nonsolvent-induced phase separation technique was exploited and the polymeric precursors were carbonized. The PIM-based hierarchically structured carbons mainly consisted of microporous domain ($\sim 7.6\text{\AA}$) and meso- and macropore. The obtained material exhibits a considerable surface area ($\sim 2100\text{ m}^2\text{ g}^{-1}$), high electrical conductivity (150 S cm^{-1}), high specific capacitances (363, 261, and 200 F g^{-1} in three-, two-electrode aqueous systems, and two-electrode organic systems, respectively) at 1 A g^{-1} , and exceptional specific energy of 43.2 Wh kg^{-1} at a specific power of 1.25 kW kg^{-1} , featuring a pore size gradient in the surface normal direction.

Key Words : Hierarchical carbons, Supercapacitor, Polymers of Intrinsic Microporosity, Nonsolvent-induced Phase Separation

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Thursday, 22/Aug/2019 12:42pm - 12:54pm

Abstract ID: 432 / FLNM-2: 9

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nano-optics, Nano-optoelectronics, Nano-Photonics and Nano-photonics

Keywords: Polyhedral Boranes, Nano, Fluorescence, Redox, Electrochromism

Pseudo-spherical Organic-inorganic Hybrid Nanomolecular Clusters Exhibiting Redox-controlled Fluorescence Switching and Electrochromism

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Polyhedral borane anions exhibit remarkably high thermal stability and resistance to oxidative degradation. Such is especially true for the twelve-vertex closo-dodecaborate [B₁₂H₁₂]²⁻, as well as the ten-vertex closo-decaborate [B₁₀H₁₀]²⁻. The stability of these clusters is owing to the extensive delocalization of their framework bonding electrons, giving rise to three-dimensional aromaticity. Substitution of these clusters with aromatic ligands was previously limited in scope. However, we recently reported new and extensive polysubstitution chemistry for these ions, where up to ten of the B–H vertices may be replaced with phenyl, substituted phenyl, or polycyclic aromatic ligands through the formation of stable boron–carbon bonds. The resulting products are pseudospherical organic-inorganic hybrid nanoparticles, which possess ligand size-dependent diameters ranging between 1.3–3.5 nanometers.

These nanomolecular clusters exhibit interesting photophysical and electronic properties, including high solution-phase fluorescence quantum yields, large Stokes shifts, and high molar absorptivities. Additionally, several of these clusters exhibit reversible redox processes. The spectroscopic and redox properties of these clusters depend on the composition of the ligand, and these may be tailored through chemical modification of the particle surface. Furthermore, the fluorescence emission, excitation, and absorption spectra for several of these species remarkably and reversibly change upon the oxidation of the boron cage from closo- to hypercloso-, thus exhibiting redox-controlled fluorescence switching and electrochromism. This study suggests that these new nanomaterials may be useful for applications in biomedical imaging and sensor development.

Abstract ID: 433

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Enzymes and Biocatalysts

Keywords: Graphene, CotA Laccase, Magnetic Nanocomposites

Efficient Cota Laccase Immobilization on Magnetic Graphene Oxide Sheets for Enhancing Biocatalysis

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In the recent decades, massive industrial revolution of textile dyes brought a serious environmental pollution, especially for water. Synthetic dyes gave warning not only for the environment but also for human health because of their existence in wool, textiles, papers, and leathers. As environmentally friendly biocatalysts, laccases can degrade a broad range of industrial toxic contaminants [1]. However, the industrial applications are limited due to the low stability and poor reusability of free laccases. Enzyme immobilization can reduce the restrictions by increasing the stability, durability and realizing continuous operations. Up to now, laccase has been successfully immobilized on various kinds of carriers, such as microspheres, nanoparticles, nanofibers and membrane. Among these carriers, the functional magnetic particles can be produced by immobilization of an affinity ligand on the surface of prefabricated magnetic beads, which can be quickly separated from the reaction medium and controlled by applying a magnetic field [2, 3]. As a result, the catalytic efficiency and stability properties of the enzyme can be greatly improved. In the current study, the functionalized magnetic graphene oxide (MGO) chelated with Cu^{2+} was synthesized. The Cu^{2+} -chelated MGO (MGO- Cu^{2+}) exhibited the highest adsorption capacity of 177 mg/g-support for CotA laccase among all synthesized nano-composites. The maximum activity recovery of laccase using MGO- Cu^{2+} was 114%. The catalytic properties of MGO-Cu-CotA laccase were significantly improved in comparison with those of free laccase. MGO-Cu-CotA laccase showed efficient decolorization rate for Congo red reached 100% after 5 h reaction at 60 °C and pH 8. MGO-Cu-CotA laccase retained 89.4 % of its initial activity after 10 consecutive cycles. These MGO- Cu^{2+} supports provide great potential for large-scale laccase immobilization in practice. [4]

Wednesday, 21/Aug/2019 4:36pm - 4:48pm

Abstract ID: 434 / FBB-2: 4

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Lab-on-a-chip

Keywords: Digital microfluidics, fluorescent pH sensor, luminescent oxygen sensor, temperature sensor, microimaging, microfabrication of multilayer materials

Multilayer lab-on-a-chip materials for simultaneous digital microfluidic operation and optical chemical sensing and imaging

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Digital microfluidics (DMF) is a favorable technology for miniaturization of laboratory procedures that uses microelectrodes and electrowetting for automated movement of droplets on very small scales. In order to make full use of its potential integrated monitoring of process parameters and reaction progress is highly desirable. Optical chemical sensors are preferred tools since they are capable of imaging analytes and process parameters spatially resolved.

Here we present results on the microfabrication of multilayer materials containing both integrated microelectrodes and auxiliary layers for DMF function and thin film optical sensor layers for integrated monitoring and their application in temperature monitoring and cell culture. We created DMF chips with dissolved oxygen (DO), pH and temperature sensors.

The DMF (bottom plate) assembly was made on a glass substrate via multiple chromium and parylene deposition, etching and stripping steps. An oxygen sensor was constructed on top of this via spin coating a 200 nm thin layer of Platinum-tetrapentafluorophenylporphyrin (PtTFPP) in Hyflon AD 60 fluoropolymer. pH sensor spots were created from fluorescein-modified pHEMA using plasma etching or lift off of a glass/electrode DMF top plate assembly. Temperature sensors were applied as CsPbBr₃ quantum dots (CsPbBr₃-QD) in fluoropolymer matrix. First applications of the multifunctional devices are shown in bacterial cell culture and temperature monitoring of electrode processes.

Fig.1: a) Image of a DMF chip with oxygen sensor and schematic layer diagram, b) Calibration curve of the oxygen sensor PtTFPP in Hyflon AD60, c) Calibration curve of the pHEMA-based sensor, d) Calibration curve of the QD temperature sensor in Hyflon AD60

Abstract ID: 435

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Green Composites

Keywords: Biosynthesis, *Cotyledon orbiculata*, antimicrobial activity

The characterization and determination of Zinc Oxide, Silver and Silver-Zinc Oxide nanoparticles exposed to extracts of *Cotyledon Orbiculata* and their antimicrobial activity in wastewater

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This study showed that the use of bottom-up method for exposing nanoparticles, such as ZnO, Ag, 3% w/w Ag-ZnO, 5% w/w Ag-ZnO and 7% w/w Ag-ZnO, to medicinal plant *Cotyledon orbiculata* enhances capable properties of the nanoparticles that can be used against bacteria. Characteristics of these nanoparticles was carried out by Scanning Transmission Electron Microscopy (STEM) technique. The STEM images obtained confirmed that the nanoparticles are within a nanometre range. Metabolites found in plants play a role in the size and shape formation of metal nanoparticles as shown by the irregular rod-like structures of 5% Ag-ZnO and 7% Ag-ZnO nanoparticles. The sizes of the nanoparticles used in this study range from 20 nm to 200 nm. Different concentrations were prepared by weighing various mass and all the nanoparticles showed antimicrobial activity against *S.aureus*.

Abstract ID: 436

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Applications of Composites

Keywords: polyaniline (PANI), polymer, biosensor, conductive polymer, matrix composites

Size-controlled Polyaniline (PANI) Nanofibers for Biosensor Application

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Intrinsically conductive polymers, polyaniline (PANI) nanofibers have attracted great interest because of their unique characteristics, such as electric properties and large surface areas and environmental stability, which have many potential applications, such as in batteries, electronic devices, bio/chemical sensors, and chemical sensors.¹⁻²

Among various intrinsically conductive polymers, polyaniline (PANI) synthesized by a rapid mixing of the aniline monomer and the ammonium persulfate initiator preventing the overgrowth of polyaniline, provide an interesting nanostructure from the standpoint of biomolecule immobilization.³ PANI themselves are conductive nanofibers and provide porous inter-fiber matrix, the size control of PANI nanofibers is still a challenge, due mainly to the less monodisperse distribution of the size and shape of the PANI polymer chains. We developed effective way to control the sizes of the PANI nanofibers, which results in controlling the polymerization temperatures from room temperature to -80 °C. The size-controlled PANI structure by temperature offers immobilized biomolecule and intimate contact between porous conductive network as well as various size-dependent chemical response for effective diagnosis platform. The size-controlled properties of the resulting PANI nanofibers, such as molecular weights, optical properties, and electron conductivity, have been demonstrated.

By systematically tailoring the size in the polyaniline (PANI) nanofibers, electron conductivity in the composite architecture is optimized to deliver appropriate sensitivity, which represents a critical step forward toward practical sensor applications. This study offers a promising route to greatly enhance the biosensor using porous inter-fiber matrix and provides suggestive insights for selection and detection of various sized chemicals for effective diagnosis.

Abstract ID: 437

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: cobalt nanoparticles, anti-microbial activity, Bacillus subtilus

The Synthesis and Characterization Cobalt Nanoparticles and their Anti-Microbial Activity against Selected Waterborne Pathogens

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Different types of cobalt nanoparticles have been synthesized in this study using wet synthesis methods. These materials were then characterized using scanning electron microscopy (SEM), energy-dispersive X-ray (EDX), Fourier transform infrared spectroscopy (FTIR), ultraviolet visible spectroscopy UV-Vis and thermal gravimetric analysis (TGA). In this study, we also report the anti-microbial activity of these nanoparticles. The bacteria used includes: Escherichia coli, Klebsiella pneumonia, Bacillus cereus, Bacillus subtilus, Staphylococcus aureus and Pseudomonas auriginosa.

The SEM and EDX results showed the presence of cobalt in the nanoparticles. The cobalt was found to be well dispersed on the morphology of nanoparticles. SEM also showed that the particles were in the nanosize range (1–200 nm). FTIR and UV-Vis Spectroscopy showed the different absorption band and peaks of the nanoparticles. The resulting nanoparticles also showed good anti-microbial activities against selected microbial contaminants.

Abstract ID: 438

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Enzymes and Biocatalysts

Keywords: Laccase, Fermentation, Magnetic Nanocomposites

Laccase: large-scale fermentation and direct capture by functional magnetic nanoparticles for enhancing biocatalysis

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Laccase, belongs to a well-studied family of copper-containing blue oxidases, which are mainly produced by fungi. The major role of laccase in lignin and phenolic compound degradation has attracted significant interest in a large number of industrial applications, such as paper manufacturing, food processing, bioremediation, biosensors, fuel cells, organic synthesis, etc [1-3]. In the current study, laccase fermentation was successfully scaled up to a 2 m³ stirred-tank reactor, and a promising farnesol addition strategy was developed to enhance the laccase production from *Trametes versicolor*. An emphasis is highlighted on direct capture of laccase from *T. versicolor* fermentation broth using magnetic mesoporous silica nanoparticles with metal affinity ligands. The Cu²⁺-chelated magnetic mesoporous silica nanoparticles with an average pore size of 14.5 nm provide 60.6-fold purification of laccase and 114.6% recovery yield of enzyme activity. Storage stability and temperature endurance of the adsorbed laccase on MMSNPs-CPTS-IDA-Cu²⁺ increased significantly, and the adsorbed laccase retained 86.6 % of its initial activity after 10 successive batch reactions operated with magnetic separation. The immobilized laccase on the magnetic mesoporous silica nanoparticles has been developed for efficient phenol degradation. The degradation rate of phenol by the immobilized laccase was 2-fold higher than that of the free laccase, and the immobilized laccase retained 71.3 % of its initial degradation ability after 10 successive batch treatments of coking wastewater.

Thursday, 22/Aug/2019 10:00am - 10:12am

Abstract ID: 439 / FESC: 11

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: Photocatalyst, Raman, High Temperature

Structural Chemistry Study on Strontium Tantalate Photocatalysts for Their Water-Splitting Properties: (2) High-Temperature Ultraviolet Raman Spectroscopy

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According to our diffraction study described in the presentation (1), photocatalytic water-splitting performance on Sr₂Ta₂O₇ is effectively enhanced by the elemental substitution introducing the electronic field in the bulk crystal structure without a large deviation of bond angles of Ta-O-Ta from 180°. In this study, we discuss strength of chemical bonds related to such structural distortions by Raman measurements.

Strength of chemical bonds in the substances can be estimated by in-situ observation of the Raman spectra at high temperatures. Here, high-temperature Raman spectra up to 1773 K were successfully observed by using UV laser to diminish the influence of thermal emission on the background intensity of the spectra at high temperatures.

The in-situ observation at high temperatures enabled each Raman band to be assigned to vibrations of internal or external bonds of TaO₆/NbO₆ octahedra. For Sr₂Nb₂O₇, one of the related compounds of Sr₂Ta₂O₇, the strength of the internal Nb-O bonds in NbO₆ octahedra was as weak as the external bonds. The weak Nb-O chemical bonds induce the large distortions of the NbO₆ octahedra and the static displacements of Nb ions from the gravity center of six O ions in the NbO₆ octahedra. They are as crucial as the static NbO₆ octahedral tiltings to decide a deviation of the Nb-O-Nb bond angles from 180°. The deviation leads to a decrease in electron migration and would decrease the photocatalytic performance. On the other hand, for unsubstituted and Ba-substituted Sr₂Ta₂O₇ for Sr, the strength of the internal Ta-O bonds in TaO₆ octahedra was estimated to be stronger than that of the external bonds. Due to the strong Ta-O chemical bonds, the dipole moments in the TaO₆ octahedra and the spontaneous polarization in the whole crystal lattice can be induced by the Ba substitution without a large deviation of the Ta-O-Ta bond angles from 180°, which enhances the photocatalytic performance. These results are consistent with our diffraction study in the presentation (1).

Both researches of diffraction and Raman experimentally demonstrated a guideline to enhance the photocatalytic water-splitting performance by the elemental substitution inducing distortions in the bulk crystal structure of the photocatalyst. One of the important keys is suppression of recombination between photoexcited electrons and holes by introduction of electric fields into the crystal, without reduction of the electron migration by controlling a degree of overlap between Ta5d-t_{2g} and O2p orbitals composing the lower part of the conduction band.

Thursday, 22/Aug/2019 9:48am - 10:00am

Abstract ID: 440 / FESC: 10

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Photocatalytic and electrochemical water splitting

Keywords: Photocatalyst, Synchrotron X-ray, Neutron

Structural Chemistry Study on Strontium Tantalate Photocatalysts for Their Water-Splitting Properties: (1) Synchrotron X-ray Diffraction and Neutron Diffraction

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Sr₂Ta₂O₇ with NiO_x cocatalyst is known as a photocatalyst, which has the high activity for overall water splitting under ultraviolet (UV) light irradiation. The activity increases about two times by Ba substitution for Sr in Sr₂Ta₂O₇, whereas it decreases to about one-half by Ca substitution. The mechanism of the changes in the activity has not yet been revealed. The larger-sized Ba or smaller-sized Ca substitution than Sr would introduce some distortions in the crystal structure of Sr₂Ta₂O₇, such as changes in the angle of the TaO₆ octahedral tilts and/or in the degree of distortions of TaO₆ octahedra. In this study, we performed accurate crystal structural analysis of the photocatalysts by Rietveld method by using synchrotron X-ray and neutron powder diffraction data.

Partial Ba- or Ca-substitution for Sr in Sr₂Ta₂O₇ increases the TaO₆ octahedral tilts and the distortions in TaO₆ octahedra, which induce dipole moments in TaO₆ octahedra and the spontaneous polarization. The electronic field in whole crystal of Sr₂Ta₂O₇ (the spontaneous polarization) and/or the local electric field around Ta ions (the dipole moments) seemingly enhance the photocatalytic activity of NiO_x-supported Sr₂Ta₂O₇ due to the suppression effect on the recombination between photoexcited electrons and holes. However, these factors cannot explain the difference between an increase in the activity by the Ba substitution and a decrease in the activity by the Ca substitution. The bond angles of Ta-O-Ta are changed by the distortions in TaO₆ octahedra as well as the tilts of the octahedra. The Ba substitution does not change the bond angles of Ta-O-Ta, while the Ca substitution makes the bond angles to deviate from 180°. The deviation of the bond angles of Ta-O-Ta from 180° prevents overlap between Ta 5d-t_{2g} and O 2p orbitals, which compose the lower part of the conduction band, and then decreases a mobility of excited electrons.

These results clearly show the photocatalytic performance is effectively enhanced by the elemental substitution introducing the electronic field in the bulk crystal structure without a large deviation of bond angles of Ta-O-Ta from 180°.

Abstract ID: 443

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Spectroscopy studies of low dimensional, nano and 2D materials Carbon Based materials

Keywords: Raman spectroscopy, PDMS, stamp, real-time, nanostructures

Real-time Raman spectroscopy of laser-ablated PDMS stamps

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Polydimethylsiloxane (PDMS) stamps provide a relatively easy yet promising new route for producing nano-scale structures. These stamps allow for micro-contact printing, where nanostructures can be cut into a master relief via laser ablation. This allows for relatively a relatively fast process of design, manufacturing, and testing of complex nanosystems. Atomic force microscopy (AFM) enables researchers to observe the topography of a sample at the nanometer scale. Tip-enhanced Raman spectroscopy lets researchers obtain relatively high-intensity, unique chemical fingerprints of samples for characterization. Here we show a process by which PDMS stamps can be cut, and then subsequently measured by AFM and tip-enhanced Raman spectroscopy. The entire process takes place on the same Raman-enabled AFM system. The samples are ablated by a laser, and then AFM and TERS tests are performed on the sample once the ablation is finished. This allows for us to observe how the ablating laser affects the PDMS surface both on a topographic and chemical level. For the first time, we can see as the laser cuts the surface how the topography changes and how the chemical structure of PDMS changes as it is exposed to the ablating laser. This study offers a new way to monitor PDMS stamp production in real-time.

Abstract ID: 444

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Dielectric, Ferroelectric and Piezoelectric materials

Keywords: Accelerated thermal ageing, Antioxidants, Breakdown Voltage, Dissipation factor, Ferrite core, High frequency, Liquid dielectric coolant, Oxidation stability, Teflon.

Influence of Soild Materials on Indigenous Natural Esters for use as an Alternate Liquid Dielectric Coolant

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Abstract: Insulation system places a vital role for normal and safe operation of any electrical system. Requirement of economic, safe, reliable and environmentally friendly insulation is need of the present day. Power systems operate at a relatively very low frequency of 50Hz/60Hz. There are also very different areas wherein transformers are required to operate at comparatively very high frequencies of about 1 kHz to 100 kHz or even more. In aircraft/defence applications, high frequency transformers are used and insulation failure can be of serious consequences therefore unacceptable. In such high frequency transformers, main insulating materials used are the liquid dielectric along with solid material such as Nomex and Teflon. Silicone fluid has been the widely used liquid dielectric coolant for airborne applications. Compatibility between the liquid dielectric and other dielectric components is very important in such applications.

In the present work, two indigenous oils codenamed as IO18 & IO19, have been investigated and their dielectric properties namely breakdown voltage, dissipation factor studied and oxidation stability measured, for use in an insulation system. The applicability of these natural vegetable seed oil/s as a liquid dielectric coolant in high voltage – high frequency transformers is addressed. The compatibility of the selected natural vegetable seed oil with the other component materials (Ferrite core, Nomex, Teflon) used in high frequency transformers is also addressed. Behaviour of each of the oil, under “as received”, treated and under accelerated thermal ageing condition is investigated. The effect on the dielectric properties namely Breakdown Voltage, Dissipation Factor and oxidation stability of the oil due to the presence of Ferrite core, Nomex, Teflon is also investigated. The effect of dissipation factor and relative permittivity on the insulating liquid for a frequency variation of 500Hz to 500 kHz is also investigated. The results were compared with silicone fluid. The results have been very encouraging indicating the suitability of the oil, as a liquid dielectric coolant, for an insulation system. IO18 has been granted with US patent. The effect of blend of both the oils as a liquid dielectric coolant is given in link paper- 2 titled “Breakdown Behaviour of Indigenous Natural Esters as a Blend for use as an Ecofriendly Dielectric Coolant”.

Abstract ID: 445

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Dielectric, Ferroelectric and Piezoelectric materials

Keywords: Key Words:Antioxidants, Breakdown voltage, Dissipation factor, Impulse Breakdown, Liquid dielectrics, Oxidation Stability.

Breakdown Behaviour of Indigenous Natural Esters as a blend for use as an Ecofriendly Dielectric Coolant

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Abstract—Natural vegetable seed oils have been in use as liquid dielectric coolants in distribution transformers. They are slowly replacing dielectric liquids mineral oil and silicone fluids which are widely used in power frequency and high frequency applications. Bio-compatibility, high biodegradability of vegetable seed oils and their high flash point (above 300°C) have contributed to worldwide efforts in developing a few of them as liquid dielectric coolants. In view of these, the present work focuses on the investigations on a blend of two indigenous oils codenamed as IO-18 and IO-19 respectively. As no specific standards are yet available for vegetable oils, dielectric parameters of silicone fluid (high frequencies) and mineral oil (power frequency) are also investigated for the purposes of comparison. Breakdown voltages (BDV) at 50Hz and BDV for different gap spacings have been investigated and results are compared with that of mineral oil. Dissipation factor and relative permittivity of the blend are investigated in the frequency range (500Hz-500kHz) and are compared with that of silicone fluid. The results have shown that the breakdown voltages of the blends are in acceptable range and in good comparison with that of mineral oil. Dissipation Factor(DF) values of the blend are found to be extremely good (low) at high frequencies and are better than the values of silicone fluid. Relative permittivity values of the blend are much better (higher) than those of silicone fluid and mineral oil. The results have been very encouraging indicating the suitability of the of the blend of the two oils, as a liquid dielectric coolant, for an insulation system. IO-18 has been granted with US patent. Further, investigations on the dielectric behavior and oxidation stability of both the indigenous oils as individual samples are presented in Link Paper 1 with title “Influence of Solid Materials on Indigenous Natural Esters for Use as an Alternate Liquid Dielectric Coolant”.

Keywords—Dielectric coolant, Dissipation Factor, Relative Permittivity, Antioxidant, Oxidation Stability.

Abstract ID: 446 / Poster: 14

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Silver nanoparticles, Activated carbon, Composite, SERS, Formaldehyde

Self-Assembling Silver Nanoparticles on Surface of Activated Carbon as SERS Substrate for Detection of Formaldehyde

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The most of efforts have been made to prepare high performance surface-enhanced Raman scattering (SERS) substrate for amplifying Raman signals. It still remains a grand challenging task in building a simple, conventional and low-cost SERS substrate with highly dense hotspots for improved sensitivity of the target analytes. We report a very dexterous strategy to fabricate a distinctive SERS substrate with high density hotspots, using common adsorbent activated carbon (AC) as template to assemble silver nanoparticles (Ag NPs). It can be estimated that the enhancement effect of Ag NPs/AC substrate is about 6-fold that of bare Ag NPs. Different from the resonant dyes, however, formaldehyde (FA) is a Raman-inactive molecule even though enhanced. Considering that, a novel method for quantitative analysis of FA using the Ag NPs/AC substrate has been developed, based on the catalytic effect of trace FA on the oxidation of malachite green (MG) through bromate in the acidic condition. The change of MG from reduced form into oxidized leucomalachite green (LMG) results in the quench of Raman signals of MG, responding to 0.07 ppb FA that is about 2 orders of magnitude lower than the limit defined by the Nash's method as a standard procedure recommended in Europe, Japan and China. Moreover, SERS examinations of endogenous FA in human urine signify that the proposed method had high selectivity, reliability and accuracy. Thus, as-fabricated Ag NPs/AC system is adequate as inexpensive and versatile SERS substrate utilized in the quantification of trace targets in various complicated matrix.

Thursday, 22/Aug/2019 11:12am - 11:24am

Abstract ID: 447 / FTF: 2

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin films in Energy Harvesting and Storage

Keywords: Graphene, Layer-by-layer, Nano, Energy Harvesting, Triboelectric, Thermoelectric

Layer-by-Layer Assembled Graphene Multilayers: Applications for Flexible Energy Harvesting Generators

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Recently, with the miniaturization of electronic devices, problems with regard to the size and capacity of batteries have arisen. Energy harvesting is receiving significant attention to solve these problems. In particular, the thermoelectric generator (TEG) is being studied for its ability to harvest waste heat energy. However, studies on organic TEGs conducted thus far have mostly used conductive polymers, making the application range of TEGs relatively narrow. In this study, we fabricated organic TEGs using carbonaceous nanomaterials (i.e., graphene nanoplatelet and single-walled carbon nanotube) with polyelectrolytes via layer-by-layer (LbL) coating on polymeric substrates. The thermoelectric performance of the carbonaceous multilayer structure was measured, and it was confirmed that the thermoelectric performance of the TEG in this study was not significantly different from that of the existing organic TEG fabricated using the conductive polymers. Moreover, by simply changing the electrolyte, p- or n-type TEGs could be easily fabricated with carbonaceous nanomaterials via the LbL process.

Triboelectric nanogenerators (TENGs) are also a promising next-generation mechanical energy harvester because of their light weight, portability, and eco-friendliness. However, some requirements such as cost-effectiveness, high performance, scalability, and simple process make the real industrial applications of TENGs difficult. In this study, we first reported graphene-based TENG LbL technique that enables low cost, durable, scalable, and wearable TENGs. The LbL-based graphene multilayer was deposited on a flat, undulated polymer substrate or textile structure, where the graphene multilayers role as a positive triboelectric-material and electrode of devices. A graphene multilayer on a textile was demonstrated for scalable and wearable TENG operated by a single electrode mode. The simple and versatile graphene-based LbL assembly can provide some portable microelectronic applications like self-powered wireless sensors and further wearable energy harvesting devices.

Abstract ID: 448

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nano-optics, Nano-optoelectronics, Nano-Photonics and Nano-photonics

Keywords: Damping of LSPR, Metallic nanoparticles, Transmittance, Photocatalysis

Strong Damping of the Localized Surface Plasmon Resonance of Metal Nanoparticles and its Applications

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Strong localized surface plasmon resonance (LSPR) of metallic nanoparticles has been proved to have the ability to effectively enhance the Raman scattering, the visible light absorption and the photoluminance emission of organic molecules and has thus got widely applications. Recently, strong damping of the LSPR of metallic nanoparticles [1] is drawing increasing attention due to the transient transition of hot electrons. We fabricate samples whose LSPR is strongly damped [2-3] and we explore the LSPR damping induced improvement of transmittance of dielectric/nanoparticles/dielectric layers [2] and the LSPR damping induced visible light photocatalytic efficiency of nanoparticles [4].

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Abstract ID: 449

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Carbon and metal oxide based composite materials

Keywords: Carbon nanotube, TiO₂, Nanoparticle, Composite, Fiber

The nanohybrid fibers composed of TiO₂ nanoparticles and carbon nanotubes for sustainable mechanical properties under harsh conditions

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Carbon nanotube (CNT) has been extensively investigated owing to its fascinating physicochemical properties such as chemical inertness, light-weight, high mechanical strength and electrical conductivity. During last decades, numerous efforts have been devoted to developing an efficient fibrous spinning process of CNT for the practical applications to automobile, defense and aerospace industries. Therefore, there were several successful spinning processes such as direct spinning, liquid crystal spinning and forest spinning. Among them, the direct spinning process is being considered as a promising approach for industrial applications owing to its compatibility with continuous and large-scale production of CNT fibers. For the practical applications of CNT fibers, it is an urgent issue to improve the long-term stability of their mechanical properties. TiO₂ nanoparticles are well known as an effective UV protective material owing to their high UV absorption, eco-friendly and chemically stable properties. Herein, we describe an efficient method to incorporate TiO₂ nanoparticles into directly-spun CNT fibers to improve their long-term stability under UV exposure. UV protective effect of TiO₂ nanoparticles on the mechanical properties and chemical structures of CNT fibers was systematically investigated as a function of UV exposure time. Based on the studies, we found that incorporation of TiO₂ nanoparticles into CNT fibers resulted in a considerably increased long-term stability of their mechanical properties by preventing formation of UV-induced defects.

Abstract ID: 450

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Biodetection

Keywords: carbon dots; aptamer; adenosine triphosphate; graphene oxide; fluorescence resonance energy transfer

Highly sensitive and selective determination of adenosine triphosphate based on fluorescence resonance energy transfer between carbon dots and graphene oxide

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Adenosine triphosphate (ATP) is a universal energy source in vivo, at the same time it is significant to the evaluation of food quality and safety [1]. In this work, we developed a novel aptasensor for detection of ATP based on biocompatible carbon dots (CDs) and graphene oxide (GO). The resultant CDs-aptamer acted as the energy donor and molecular recognition probe. It can be adsorbed onto the surface of GO which served as the energy acceptor through π - π stacking and hydrophobic interaction, and the fluorescence of CDs-aptamer was effectively quenched via strong fluorescence resonance energy transfer (FRET) between CDs and GO. In the presence of ATP, it combined with the aptamer and the CDs-aptamer was desorbed from GO due to the conformational change [2], which significantly hindered the FRET and the fluorescence of CDs recovered. Under the optimal conditions, the detection limit of the proposed aptasensor was 0.08 nM with linear range of 0.10-5.0 nM. In addition, the aptasensor exhibited several advantages compared to previous methods: (1) All materials used in this work are cheap, available and eco-friendly. (2) The aptasensor shows good sensitivity and selectivity. Furthermore, the present method was successfully applied to the determination of ATP in yogurt samples and can also be extended to the detection of other targets with a selection of corresponding aptamers.

Abstract ID: 451

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Metal oxide, carbon, nitrides etc based thins Films

Keywords: Titanium dioxide, Thin Film, Sensing materials

Titanium suboxides synthesis by direct oxidation method

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Titanium oxide is well known material with well defined properties and applications. Scientific community are now interested in modification of this material with purpose to change properties and extend applications of titanium oxide [1]. It can be done by incorporation of various atoms or by forming different stoichiometry's titanium oxides. Both ways are challenging due to necessity of high temperatures and highly pure gas atmospheres during synthesis [2,3].

This research is dedicated to show a simple technology for controllable composition of titanium suboxides synthesis from the aqueous solutions in order to extend materials of titanium oxide applications due to such properties as significantly lower band gap and nanoplatelet-shaped morphology. Investigation was made both with particles and layers. In order to prove the formation of suboxides, EPR and XRD we employed. Ellipsometry was used to measure the thickness and band gaps of the films. It varies from less than 3,2 eV to 1,29 eV depending on the oxide composition. The modelling was also used for calculations the porosity of layers showing that porosity is nearly 80%, what could be very important for application of these products in the gas sensing. All these results were achieved by applying hydrothermal synthesis without any need to use high temperatures or highly pure inert atmosphere during synthesis.

Abstract ID: 452

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Piezotronics for smart systems

Keywords: PLZST, Antiferroelectric, Pyroelectric, Single Crystal

Energy harvesting properties and device of PLZST antiferroelectric single crystal

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(Pb,La)(Zr,Sn,Ti)O₃(PLZST) antiferroelectric(AFE) materials with complex perovskite structure have rich phase transformations when applied an external stimuli, such as electric field, temperature, stress, etc. The phase transformations generally involve development/release of polarization, strain, dielectric, electrocaloric and pyroelectric properties, which makes the PLZST system very promising for high-sensitive actuators and transducers, solid-state cooling and pyroelectric detectors. Structural phase transitions, thermal–electrical energy harvesting and electrocaloric properties of the PLZST crystals with (100)c, (110)c, and (111)c were investigated. The pyroelectric response temperature ranges could be broaden up to 70 °C. This broaden pyroelectric response temperature range stems from the depolarization process of multiple engineered domain configuration in poled single crystals. Prototype pyroelectric devices based on the PLZST AFE single crystals with compositions near MPB were fabricated. The devices have a quick response time and high output voltage, and the maximum output voltage of the device based (111)c PLZST single crystals was 120 V. The results demonstrate the competence of PLZST single crystals for pyroelectric energy harvesting and provide new opportunities to improve the energy harvesting density by anisotropic structural layout.

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Abstract ID: 453

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Manufacturing and formation techniques

Keywords: Fullerenes, Conducting Polymers, Energy Storage

**Polypyrrole Nanoparticles Doped with Fullerene and Fullerene/Pd Coordination Polymer
Uniformly Distributed in the Polymeric Phase**

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Composites of polypyrrole-fullerene C60 and polypyrrole-C60/Pd coordination polymer were prepared by the introduction of fullerene during polymerization of pyrrole initiated by the oxidation of pyrrole oligomers with C60. Composites were precipitated in form of spherical particles and their sizes ranged from 20 to 400 nm depending on the time of polymerization. In the case of polypyrrole-fullerene composite, C60 nanocrystals with approximate size of 1 nm were uniformly distributed within the polymeric material (Figure 1). The C60/Pd polymeric material is less uniformly distributed within the pyrrole in the composite. The amount of fullerene or coordination fullerene polymer incorporated into polypyrrole depended on the C60 concentration in the solution used for the composite formation. In both composites, the partial charge transfer between polypyrrole chains and fullerene moieties takes place. The composites were electrochemically active over a large potential window. At negative potentials, fullerene moieties were reduced. In the positive potential range, polypyrrole chains were oxidized. Both processes were accompanied by complex ion transfer between supporting electrolyte solution and composite solid phase immobilized at the electrode surface. These composites can be used as electron transporting materials in solar cells. The advantages of this material over crystalline fullerene films or domains are its higher electron conductivity due to the partial charge transfer between the polypyrrole and fullerene nanocrystals or fullerene coordination polymer, high concentration of fullerene units and composite stability.

Abstract ID: 454

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Synthesis, Controllable Growth and Characterizations

Keywords: Nanowires, Doping, Characterization

Investigation of effect of lithium doping in silver nanowires

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Silver nanowires have several important applications such as catalysts [1], bio-nanosensors [2], and high conductivity electrodes [3]. Doping silver nanowires with lithium could lead to increase the mechanical strength and conductivity. It has been shown that ultra-light weight alloys with high strength is crucial for next generation industrial applications [4]. Although it is a promising candidate, it is a big challenge to introduce lithium into silver nanowires. In this work, silver nanowires have been successfully synthesized by adding different concentrations of lithium nitrate to the PVP solution by a simple solvothermal method, by varying lithium mass percentage of 0, 1, and 3 %. The typical size of a nanowire is about 50 nm in diameter and 20 micron in length. We noticed a slight decrease in diameter once doped with lithium elements. We performed XRD on the nanowires and did not notice a new peak; however we observed a systematic shift of one of the peaks (220). Absorbance was measured by UV-visible-absorbance spectrometer and Raman spectroscopy was performed by 488 nm laser excitation. In the light of XRD data, lithium is believed to be introduced into the structure. There is a decrease in the peak position of (220) peak as well as an increase in the intensity while we increase the lithium concentration. UV-visible absorbance data showed two major peaks around 350 and 390 nm which are attributed to the plasmon resonance peaks of silver. The peak intensities increase with increase of lithium doping. In addition, the absorption peak undergoes a blue shift of about 15 meV at 3 % lithium doping compared to no lithium doping, which could be understood as lithium incorporation into the silver nanowires. Furthermore, the Raman data revealed a new peak in silver nanowires spectrum which could be due to the interaction between lithium and silver atoms.

Key Words: Nanowires, Doping, Characterization

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Abstract ID: 455

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Industrial applications of composite materials

Keywords: polyolefin, rheology, extrusion, thermoforming, film

Influence of Melt Blending on Controlling of Defects in Polyolefin Melt Processing

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Polymer melt processing operations such as extrusion film casting (EFC) or plus-assist thermoforming (PAT) are commercially important techniques that are used to produce several thousand tons of polymer films/coatings/thermoformed products on an industrial scale. However, these processes suffer from critical defects that limit the productivity of such operations. In particular, in EFC, defects such as necking (inhomogeneous reduction of film width) and edge-beading (thickening of film edges) are interrelated and are influenced by both material & process parameters. In PAT, the final thickness distribution of the part is highly influenced by the sheet sag. In general, linear chain architecture polyolefin resins such as linear low-density polyethylene (LLDPE) or high-density polyethylene (HDPE) are not amenable for EFC or PAT based processing since they do not possess the key melt rheological properties such as strain hardening in melt extension. In the present research we are interested in understanding how macromolecular chain architecture (for example containing long-chain branching or LCB) &/or molecular weight distribution (MWD) influences the necking behavior and sag resistance of viscoelastic melts in the EFC & PAT processes, respectively. We have used commercial polyethylene (PE) resins of both linear chain & long chain branched molecular architecture to produce blends in appropriate ratios and then used the blends in producing extrusion cast films or thermoformed products under controlled experimental conditions. All the materials are characterized for their macromolecular properties such as moments of molecular weights, long-chain branching, etc. Additionally, the resins are also extensively characterized rheologically under both steady and dynamic conditions wherein transient extensional and shearing properties are measured. The necking profiles of the films are imaged and the velocity profiles during casting are monitored using particle tracking velocimetry (PTV) techniques. The final thickness distribution of PAT products is also quantified under various processing conditions. We present results that demonstrate that the extent of necking of the PE films or the final thickness distribution of PAT products is highly influenced by our polyolefin blend properties.

Abstract ID: 456

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Fuel Cells

Keywords: Metal-organic frameworks (MOFs), acid mine drainage, PET bottles, hydrogen storage

Holistic approach for low-cost synthesis of Fe-based Metal-organic frameworks (MOFs) using Fe derived from acid mine drainage and PET-derived organic linker

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Metal-organic frameworks (MOFs) have emerged as one of the most promising materials for wide-scale applications that include, gas storage, drug delivery, water treatment, and catalysis, among others. However, due to the high cost of synthesis feedstocks together with low maturity of MOFs production technology, there has been low commercialization effort of MOF materials and related technologies [1]. Therefore, the current study aimed at employing the utilization of unconventional metal feedstock and organic linker source to develop a method that will contribute in lowering the cost of producing MOFs. In this case, Fe-rich acid mine drainage, which is a waste water stream generated from abandoned and active mining activities, was utilized as a source of the Fe metal. On the other hand, a popular organic linker (terephthalic acid) was obtained from the depolymerisation of waste Polyethylene terephthalate (PET) bottles [2]. The two wastes were utilized to crystallize Mil-101 (Fe) MOF. The obtained MOF was characterized and compared to that obtained when virgin chemical feedstocks were used during the synthesis process. Furthermore, the resulting Fe-MOF was tested for hydrogen storage applications. The obtained results show that the performance of the resulting MOF was not highly compromised when unconventional synthesis feedstocks were utilized and hence the adopted holistic approach has a high potential for contributing towards reducing the cost of producing MOF materials.

Abstract ID: 457

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Nanostructured materials for advanced batteries

Keywords: SPS, Nano, Sol-Gel, Thermoelectric

Preparation Nano powder perovskite ceramics and sintering with SPS technique

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Sintering Plasma Spark (SPS) is advance technique that applies pressure and pulse electrical energy to sintering powder functional material of solid to achieve highly dense and homogeneous Nano-structural.

This method has ability to produce, sensors, capacitor, semiconductors, Bio-medical materials and different kinds of advanced new materials in a minimal sintering time and grain size than conventional methods. Power consumption is reduced about one third to one fifth compared to other sintering techniques such as pressure-less sintering, hot press and hot isostatic pressure sintering.

One of the important point to develop this method use suitable powder material, in this paper sol-gel technique used to make perovskite powders and powder sintered with the SPS method, permittivity Barium Strontium Titanate (BST) such as thermoelectric material tested, the result shows sharp peak near room temperature can obtained with 5 percent Strontium Titanate solution during producing Nano-powder, with this method curie temperatures can easily shifted

Abstract ID: 458

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Applications of low dimensional, nano and 2D materials

Keywords: Nano, Fano resonances, interference of electron waves

Fano resonances at interference of electron waves in geometrically inhomogeneous semiconductor 2D nanostructures

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Fano resonances (FRs) in a semiconductor 2D nanostructure (NS) geometrically inhomogeneous along the propagation of the electron wave (the x axis) and symmetric along the z axis (the z-axis is the dimensional quantization axis) are theoretically investigated. As is known, FRs [1] arise from interference of electron waves propagating along two channels: one of them in the continuous energy spectrum, and the other - a quasistationary state against the background of this spectrum. The considered NS consisted of three sequentially arranged rectangular quantum wells (QWs) in which the motion of the particle was limited only along the z axis: QW1 of width L_1 at $x < -a$, QW2 of width L_2 at $-a < x < a$ and QW3 of width L_1 at $x > a$. It was assumed that $L_1 < L_2$. In this case, the potential along the x-axis abruptly changed at the points $x = -a$ and $x = a$, and in each QW a series of quantum-size subbands was formed. Thus the energy subbands $E(1),n$ in QW1 and $E(3),n$ in QW3 was the same for the same width of this QWs. In a wide QW2 the distance between subbands $E(2),m$ was less than the distance similar number of subbands in QW1 and QW3 (figures 1,2,3 in round brackets indicate the number of the QW, and n and m – number of subbands, respectively, in QW1, QW3 and QW2). Therefore, in QW2 formed longitudinal rectangular QW along the x- axis of width $2a$, due to the different energy position of the subbands in QW1, QW3 and QW2. These QWs also formed quantum-size subbands $E_x(2),t$ due to the restriction of motion in them along the x-axis. These subbands were the quasistationary states providing the formation of FRs in the considered nanostructure. We calculated the dependence of the nanostructure transmission coefficient $|T(E_x)|^2$ for the electron wave of the unit amplitude propagating from the QW1 along the lower subzone $E(1),1$, on its longitudinal energy E_x in the range $E(1),1 < E_x < E(1),2$. The widths of the QWs L_1 and L_2 in the symmetric on the z-axis NS were chosen so that in this range of variation of E_x in QW2 there exist at least two longitudinal QWs of different depths with quasistationary states: $QW_{x,1}$, formed by the subbands $E(1),2$, $E(2),2$ and $E(3),2$, and lying higher in energy $QW_{x,2}$, formed by the subbands $E(1),2$, $E(3),2$ and $E(3),2$. In this case, the wave propagation to QW2 was possible only through this overlying subband, since the transition from the subband $E(1),1$ in QW1 to the $E(2),2$ subband in QW2 was forbidden by the symmetry of the NS. At the same time, the wave propagation in the channel in the continuous spectrum and in the quasistationary state with the corresponding energy was possible in QW2. Further, the interfering waves propagated in QW3 also along one lower subband with energy $E(3),1 = E(1),1$. Thus, when changing E_x , depending on $|T(E_x)|^2$, FRs appeared.

Key Words: Nano, Fano resonances, interference of electron waves

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Abstract ID: 459**Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)****Poster Presentation**

Topics: Fundamental investigations on low-dimensional nanomaterials and their functional structures properties

Keywords: Silica glass, Ion implantation, Quantum dots, Intrinsic defects

Planar photonic structures based on Gd-implanted silica glasses and films

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Ion implantation into SiO₂ host matrix has been receiving considerable attention of materials scientists because it is a powerful method to re-build the electronic structure and physical properties of this practically significant wide-gap transparent insulator for optoelectronic applications [1]. Gadolinium ion is promising due to all Gd³⁺ energy levels of excited states are located in the ultraviolet (UV) spectral region, which is of interest for new photonic devices and radiation energy converters. The main goal of present work is to obtain the information about electronic structure and optical properties of glassy SiO₂ matrixes implanted with Gd³⁺ ions at different fluences. The first task is devoted to determining the structural states of ion-implants with accounting of different embedding scenarios (clusterization, oxidation, formation of new microphases). The second task of the study is related with analysis of changes in atomic and matrix energy structure induced by ion radiation impact and following thermal treatment. A special attention is paid to relationship «atomic disordering-electronic structure-optical properties».

Electronic structure and optical properties of silica glass implanted with Gd-ions were studied by combined experimental (XPS, optical absorption) and theoretical (DFT-modeling) approaches. Analysis of the electronic states of Si and O proved by the XPS technique indicates the fabrication of ≡Si–O–[Gd]³⁺... complexes in as-implanted samples. Thermal annealing activates the migration of Gd at the Si position with the passivation of oxygen atoms and appearance of oxygen-poor silicon. DFT calculations of the most energy-efficient scenarios for Gd-embedding in silica confirmed that Gd is located in the interstitial and substitutional positions for as-implanted and annealed samples, respectively. Optical absorption of Gd-implanted silica in the spectral region of band tails obeys the «crystal-like» Urbach rule, the parameters of which reflect the degree of structural disorder. Ion implantation induces the «quasi-dynamic» disorder, while the thermal treatment causes a partial ordering of the structure. Optical gap for direct interband transitions as well as the effective energy of phonons, that are responsible for temperature shift of the fundamental absorption edge, decrease after both radiation treatment and thermal annealing. The main reason for this is the change in the local atomic displacements.

The photoluminescence spectra at low temperatures (8 K) showed the presence of a new type of optically active ODC centers modified by gadolinium (the luminescence band is 2.2 eV). With an increase in fluence, a luminescence band of 1.8 eV is observed, which is characteristic of silicon quantum dots [2]. The destruction of Si – O bonds and the subsequent clustering of oxygen-deficient Si atoms leads to the formation of silicon nanocrystals: [≡Si – Si≡] ... [≡Si – Si≡] → Si QDs.

Abstract ID: 460

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin Film Growth & Epitaxy

Keywords: Cesium iodide, Fractals, Self-similarity, Crystallization

Orthogonal fractal growth of CsI domains forming a ladder-like structure

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A unique structure of a thin layer consisting of cesium iodine, manifested by a “ladder-like” fractal structure formed by spin-coating is reported herein. The ladder-like structure is made of mm-size domains, each comprising of a highly correlated, perpendicularly interconnected, network of CsI lines. Each line served as the growth origin of 2-3 levels of short, perpendicularly-oriented CsI crystals, yielding a fractal dimension of 1.53. The observed structure differs from common Diffusion Limited Aggregation (DLA) shapes by the absence of any morphological indicators that may point on the origin of growth. Furthermore, the perfect orthogonal alignment of all junctions in the CsI structure is very rare in DLA type of growth. A formation mechanism is presented, based on studying the evolution of this structure at different spinning rates and on a variety of substrates. It is proposed that this unique structure originates from a rare combination of conditions: strong anisotropy in surface energy between different facets arising from the primitive ionic crystal of CsI, the strong water-breaking property of cesium ions and an unusual effect of mesoporous substrates in preventing premature nucleation.

Abstract ID: 461

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Solar Cells

Keywords: Gadolinium oxide, Nanoparticles, Energy Conversion, Defects

Functional materials based on Gd₂O₃ nanoparticles for UV, VIS and IR-conversion

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Gadolinium oxide doped with rare-earth ions are of interest as a new type of material for energy conversion devices, in particular, for solar cells [1]. Improvement of functional characteristics of converters based on rare-earths requires the optimization of synthesis technologies which determine the atomic and electronic structure of materials and, ultimately, their optical properties. In present work, we summarize the basic requirements for the crystal structure type and defectiveness of Gd₂O₃ matrix as well as the concentration of dopant ions to achieve the enhanced energy conversion efficiency. Comprehensive analysis of XPS, Raman and optical spectroscopy data reveals that in cubic Gd₂O₃ point defects of anionic sublattice (oxygen vacancies) are responsible for the change in the cation energy structure and the appearance of additional Gd³⁺ electronic states in the Gd₂O₃ band gap region [2]. The Gd³⁺ ions become optically active and can be excited in the UV spectral region with the following energy transfer to the dopants. This provides an additional channel for energy conversion without deliberate introduction of donor ions into the lattice, since this role is played by host lattice cations – Gd³⁺ ions. It is especially promising for increasing the efficiency of Si-based solar cells because the additional quanta with UV energy will participate in the solar energy conversion. In monoclinic Gd₂O₃, impurity hydroxide ions arising at the synthesis stage completely quench the emission, so this polymorph is not suitable as a luminescent material, and we focused on the Gd₂O₃ nanoparticles with a cubic structure to search for the optimal Er³⁺ concentration. Optical reflection spectroscopy we found the effect of giant phonon softening in Gd₂O₃ doped with 1% of Er³⁺ ions [3]. Analysis of temperature dependence of Er³⁺ luminescence confirmed that minimal non-radiative losses are observed in nanoparticles with this concentration of activator. Minimization of thermal losses leads to enhanced quantum efficiency of erbium luminescence under UV radiation conversion.

Wednesday, 21/Aug/2019 7:03pm - 7:15pm

Abstract ID: 462 / FC: 16

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Photocatalysis

Keywords: Transient FTIR, Step-Scan, Carbon nitride, photoactive materials

Transient photoinduced phenomena in graphitic carbon nitride as measured at a temporal resolution of a few nanoseconds by step-scan FTIR

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Transient FTIR spectra of graphitic carbon nitride were measured at a temporal resolution of a few nanoseconds. Variations in the location and the intensity of specific peaks and emerging of new peaks were observed during the first 170 nanoseconds after excitation. A comparison was made between graphitic carbon nitride prepared at two temperatures: 510 °C and 650 °C. The material prepared at 650 °C revealed very strong non-specific absorption beginning 35 nanoseconds after excitation and lasting for 20 nanoseconds. This phenomenon, termed “IR-blackening” was observed neither in g-C₃N₄ prepared at 510 °C nor in g-C₃N₄ prepared at 650 °C that was exposed to hole scavengers (ethanol and benzyl alcohol). In contrast, exposure of material prepared at 650 °C to an electron scavenger (methyl viologen) hardly alter the “IR-blackening” phenomenon. The results were explained by a mechanism, predicting higher reductive activity for materials having imperfect heptazine polymerization, as indeed was found in the photocatalytic degradation of 4-nitrophenol.

Based on these results, the pros and cons of this technique as a general tool for studying localized photo induced effects in photoactive materials will be discussed.

Abstract ID: 463 / Poster: 28

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Industrial applications of composite materials

Keywords: Superhydrophobic, cementitious

Superhydrophobic Cementitious Materials

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A superhydrophobic cementitious material has recently been successfully synthesized, which consists of both an inorganic backbone that supports the material structure and organic functional groups that offer viable superhydrophobic functionality. Laboratory research was conducted to characterize the hydrophobicity of the as-prepared porous bulk solid as well as its powdery derivative (i.e., by fine-grinding) as well its microstructure, thermal and chemical stability, and its composition. Potential applications were also investigated such as acting as amendments for traditional ordinal Portland cement as well as soil amendments for tune its permeability. Preliminary results showed that efficient and proper dispersion of the micron-sized additive plays a key role for the amended Portland cement's hydrophobicity. Further testing is being conducted to determine an optimal percentage of the additive to achieve comprised yet best performance for hydrophobicity as well as strength of the cement.

Wednesday, 21/Aug/2019 4:48pm - 5:00pm

Abstract ID: 464 / FBB: 5

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biodetection

Keywords: biosensor, detection biomarkers, graphene FET, high sensitivity, physiological conditions

A universal biosensing platform based on carbon nanomembrane (CNM)/graphene heterostructures

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Chemical functionalization of single-layer graphene (SLG) is of key importance for applications in functional electronic devices such as, e.g., field effect transistor (FET) based nanosensors. However, the electronic structure of graphene is typically degraded after the functionalization, which significantly restricts the applications. Here, we present a universal route to non-destructive chemical functionalization of graphene FETs with amino terminated 1 nm thick carbon nanomembranes (NH₂-CNM) generated via electron beam induced crosslinking of aromatic self-assembled monolayers. [1-3] We demonstrate in detail characterization of the transport properties of these heterostructures and employ them for highly sensitive detection of pH-values at physiological conditions. Additional biochemical functionalization of NH₂-CNM with aptamers enables development of custom designed highly sensitive (detection limit below 1 pM) and highly selective biosensors for detection of biomarkers in clinical diagnostics [4].

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Abstract ID: 465

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Advances in Bioelectronics and Commercial biosensors

Keywords: diabetes, islets, antibody, spr, microfluidics

Affinity-Based Culture Platform for Human Hormone Profiling

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Integrating biosensors with microfluidic cell culture platforms holds much promise for characterising the mechanisms and possible therapies for diseases such as Type 2 Diabetes, though still faces obstacles in sensor reliability and platform fabrication. We developed self-assembled monolayer (SAM) on polymer surface chemistry attachment protocols for immobilizing antigens on the surface of gold microarrays, which results in a higher reproducibility of impedance spectroscopy antibody detection measurements. Translatable to other transduction methods, such as surface plasmon resonance imaging (SPRi), these recipes for immobilizing proteins on Gold films can be tailored specifically to individual hormones, allowing for multiplexing capabilities. Detecting numerous specific analytes simultaneously and in real time is a powerful tool to investigate the release dynamics of disease biomarkers produced by endocrine signalling cells. The islets of Langerhans' are clusters of cells housed in the endocrine pancreas, the dysfunction of which is indicated in the pathophysiology of Type 2 Diabetes. In addition to endocrine signals, islets also communicate via paracrine (cell-cell) interactions. A 3D cell culture platform utilizing a scaffold gives support to the cells and promotes cell communication. Islets comprise only 1-2% of the volume of the pancreas, yet they receive 10-12% of the organ's blood flow [1], hinting at their important role by their need for oxygen consumption. The scaffold structure allows for perfusion of nutrients and oxygen to the cells, ensuring that even large ensembles have proper vascularization. Combining up to date cell culture methods with cutting edge biosensing technology, the microfluidic perfusion platform mimics in vivo conditions of shear stress and fluid flow in order to maintain islet viability in vitro, allowing disease modeling, drug screening, and facilitating transplantation procedures.

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Abstract ID: 466

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Nanostructured materials for advanced batteries

Keywords: Nanogranular-compound, Green-house-Energy-storage, IR- to UV, GA/cm²

Nanogranular Compound Material Layers Serve as Storage for Infra-Red to Ultra-Violet Photons for Energy Supply of Electric Machines

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NASA's "Energy Budget of the Earth", Leob et al. J. Clim, 2009, Treuberth et al. BAMS. 2009, NP-2010-05-265-LaRC. was measured by NASA over 10 years. These measurements tell that energy from the sun and space is sent to the earth in the form of visible light during the day (In total Silicon solar cells can harvest in the day 40W/m²) and IR –radiation in the 8 μm to 10 μm (up to 340 W/m²), but sent all day and night. Nanogranular Compound Material Layers e.g like Pt/C can serve as absorbers and as storage for Infra-red to Ultra-Violet Photons for the Energy Supply of Electric Machines. Here the energy is stored in a 2-component material composed from Platinum nanocrystals of 2 nm diameter which is embedded in a nanogranular phase of Bucky balls from Carbon which embeds the Pt nanocrystals. Due to the work functions of the two composite materials, Pt : 5,4 eV, and C: 4,8 eV, the Fullerene (carbon nanocrystals) lose their electrons to the Pt crystals. Both crystals form a common Fermi level at 5,1 eV, which extends throughout the mixture of the microcrystals. This mixed material now contains Bosons, electron with hole and antiparallel spin. This allows storing a density of 1028 / cm² of Bosons. However, if an IR photon of 8 meV is absorbed by the composit, the photon can lift the electron only into the so far empty level, where electron and hole immediately combine to a Boson. Using a field gradient along the storage layer renders to move the Bosons to the end of this crystalline phase, where it releases the electron charge of the Boson as an electron to a storage device or directly to a user. The efficiency of such storage, which is at 300 K or room temperature, is 1000 times higher than the efficiency of a superconductor cable cooled to 40 K. Only a very thin cable or sheet material is required, and can be fabricated with parallel operating field emitters for the storage.

The material and its characteristics has been discovered and measured at Deutsche Telekom Research Center in Darmstadt, Germany [], and was later name protected []. By the explanation of superconductivity by Bardeen, Cooper and Schrieffer, electrons having antiparallel spin in the cooled state below 40 K can carry 1 MA/cm² current density. However in our experiments we measured at room temperature in 1994 to 2000 current densities up to 1.4 GA/cm² using Pt/C compounds. Researchers at KNMF of KIT Germany [] measured between lithographically defined Pt contact lines a current carrying capability of 0,6 A applying 4 V to a ribbon of 1 μm width and 150 nm thickness. At IVNC 2017 Koops and Rangelow showed that the Koops-GranMat® Material has 0 resistances, but the contact areas from normally conducting materials need to be large enough, not to melt the contact material []. Koops-GranMat® can carry 1,4 GA/cm²!

Thursday, 22/Aug/2019 9:12am - 9:24am

Abstract ID: 467 / FLNM: 7

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Carbon Nanomaterials

Keywords: Graphene, Humic acid, Ball mill, CNT

Synthesis of nitrogen doped graphene/carbon nanotubes nanocomposite using urea and humic acid

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A doable, low cost, and scalable method is demonstrated to synthesis graphene-carbon nanotubes nanocomposite using humic acid and urea via ball mill technique. Firstly, graphite, carbon nanotubes and urea have been milled for one hour then humic acid powder was added and annealed in Argon atmosphere for another one hour at 600°C. The structural characterizations were investigated using scanning electron microscopy SEM, Raman spectroscopy, X ray diffraction, and Fourier transform infra-red spectroscopy. The SEM measurements reveal the fluffy and highly porous morphology of the obtained powder. It has been observed that some of the carbon nanotubes were unzipped and some of them were completely opened during the synthesis process. It has been found that urea and humic acid have a crucial impact during the synthesis process. The presented method is very straightforward and can be scaled up for industrial applications.

By controlling the preparations, like ball size to powder ratio, rotating speed, CNT concentration, and operational time were investigated. it is possible to achieve significant impact in enhancing the desired properties of the synthesized nanocomposite, for further applications of humidity sensing, and supercapacitor application.

Thursday, 22/Aug/2019 8:48am - 9:00am

Abstract ID: 468 / FESC: 5

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Advances in electrolyte and electrolyte additives for energy storage devices

Keywords: Mesoporous Carbon, CNT, polymer gel electrolytes, all-solid Energy Storage

Mesoporous Electrodes and Polymer supported Electrolytes for efficiency of Electrochemical Energy Storage Devices

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Previous studies displayed that the supercapacitor electrodes possessing high surface area and rich surface chemistry contribute to energy densities and charge rapidly. New mesoporous films which are a combination of graphene, CNT and carbon complexes preferably in core-shell architectures introduce superior capacitive charge-storage properties. Moreover, the electrolytes also play an important role for the increase of the potential window but must be compatible with the electrode materials as well as sustaining environmental retention and being durable under exceptional conditions such as these at space. Low-Orbit satellites require energy harvesting systems and the rapid charging, peak power storage devices for their long-term self-sufficient decentral operation.

This work describes the fabrication and performance of the cells made of mesoporous carbon-based electrodes which are either embedded as composites or nano-structured and polymeric solid electrolytes containing integrated salts and ionic liquids.

The electrode layers are deposited by doctor-blade technique or by vacuum deposition techniques and combined with polymer based electrolytes in pouch cells. For comparison of the specific and areal capacitance values, discharge capacitance retention and charge-discharge performances, the pouch cells consisted of carbon black electrodes and ionic liquid and LiClO₄ based polymer electrolytes are manufactured and tested. The electrochemical performances, energy and power densities are calculated and compared. The cyclic charge and discharge behavior are considered in terms of discharge capacitance fading. The role of specific electrolyte and the effect of mesoporous electrode materials and conducting polymers are determined and the beneficial factors are demonstrated by means of Nyquist plots.

Abstract ID: 469

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Anodes and cathodes Materials

Keywords: 3D rod micro/nanostructure, Solvothermal method, Li-rich cathode, Li-ion battery

**Facile Synthesis of $\text{Li}_{1.2}\text{Mn}_{0.6}\text{Ni}_{0.2}\text{O}_2$ with 3D Porous Hierarchical Micro/nanostructure
by One-step Solvothermal Route**

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Li-rich layered oxides are considered to be one of the most promising cathode materials for lithium-ion batteries (LIBs). However, they are suffering from rapid capacity fading and poor rate capability. Herein, a lithium-rich layered oxide $\text{Li}_{1.2}\text{Mn}_{0.6}\text{Ni}_{0.2}\text{O}_2$ (PLMNO) with hierarchical micro/nanostructures is prepared through a solvothermal method followed by calcination process. The PLMNO material consists of primary nanoparticles with exposed {010} planes assembled into a 3D rod-like structure, which exhibits a facile pathway for the transportation of Li^+ and electrons. The initial charge and discharge capacities at 0.1C (1C=200 mA g⁻¹) are 348.3 and 263.4 mA h g⁻¹, respectively, with a coulombic efficiency of 75.6% between 2.0 ~ 4.8 V. At 1C, a much higher discharge capacity of 197.3 mA h g⁻¹ can be remained with a capacity retention of 88.5% after 200 charge/discharge cycles.

Abstract ID: 470

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Catalysis and Energy

Keywords: Hydrogen production, Ammonia borane, Catalysis, Hydrolysis

Poly(N-vinyl-2-pyrrolidone)-Stabilized Ruthenium Supported on Bamboo Leaf-Derived Porous Carbon for NH_3BH_3 Hydrolysis

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Among the various chemical hydrogen storage materials, ammonia-borane (AB, NH_3BH_3) has been considered as one of the most important promising candidates with respect to its high hydrogen capacity (19.6 wt%), low molecular weight (30.9 g·mol⁻¹), nontoxicity, high stability and environmentally benign [1-3]. In this work, poly(N-vinyl-2-pyrrolidone) (PVP)-stabilized ruthenium supported on bamboo leaf-derived porous carbon (Ru/BC) has been synthesized via a one-step procedure. The as-synthesized catalysts are characterized by means of XRD, XPS, SEM. As catalyst for hydrogen generation from AB hydrolysis at room temperature, the Ru/BC catalyst stabilized with 1 mg PVP exhibits high activity (TOF = 826.6 mol H₂·mol Ru⁻¹·min⁻¹) and low activation energy (E_a = 19.35 kJ·mol⁻¹). In addition, fair recyclability with 55.6% of the initial catalytic activity is retained after ten cycles, which confirms PVP can prevent agglomeration and stabilize Ru/BC particles. Our results suggest that PVP-stabilized Ru/BC is a highly efficient catalyst for the hydrolysis of AB.

Abstract ID: 471

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Analysis of Wood and Natural Fibre Composites

Keywords: agro-waste, nanocellulose, water filtration, polymer composite

Extraction of Cellulose from *Vitellaria paradoxa* agro-waste for possible Water Filtration Polymer Composite preparation

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The increased demand for Shea products (*Vitellaria Paradoxa*) has led to a corresponding increase in agrowaste generated. Shea nut shells (SNS) as one of the waste generated was subjected to varying compositions of chemical treatments for the possible extraction of nanocellulose. The samples collected were ground to powder, sieved and treated with 20 % alkali solution for 2 h at 80 oC. The mass to liquor ratio was varied and resulting samples were characterized using FTIR, TGA, XRD and SEM. The best treated sample was further tested for its capacity to remove selected heavy metals from water samples. From the results, the SNS contained 45 % of cellulose, the XRD and FT-IR showed that the 1:20 (w/v) ratio gave best treated samples. The amount of hemicellulose and lignin removed were highest in the sample when compared to other samples treated with 1:5, 1:10 and 1:15 (w/v). Additional treatment with NaClO₂, as bleaching agent, further removed the hemicelluloses remaining in the samples as observed in the TGA. The the selected sample was able to remove heavy metals such as Pb (38 %), Cd (42 %), Ni (25 %) and Co (44 %). It was concluded that the 1:20 (w/v) mass to loquor ratio was good but for involved result, other treatment conditions used can be optimized as all the samples still contain hemicelluloses in them. However, the combination of alkali and bleaching gave the best treatment.

Abstract ID: 472

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Structural, Electronic, Optical and Magnetic Properties

Keywords: Nanoscale MOSFET, I-V Characteristics, Energy Band Diagram

Source and Drain Under/Overlap with the Gate in 1D GAA MOSFETs and TFETs: a Better Performance

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Based on the NEGF ballistic transport simulation, optimized homojunction 1D GAA MOSFET and TFET are proposed in this article. This structure enhances the ON-state current and could extensively suppress the ambipolarity of a TFET. By changing the gate length and insulator thickness along with different values of doping levels and dielectrics of the source/drain/channel regions, a subthreshold swing SS lower than 30 mV/dec with an ON/OFF ratio of 10^8 are obtained at $V_G=V_D=0.4$ V. In this study the impact of source (drain) underlap/overlap with the gate are specially investigated in reaching an optimum result. This could help the SS of a TFET reach a value around 15 mV/dec. Such advantages can be followed on other 1D TFET devices and are explained on energy band diagram of the device.

Abstract ID: 473 / Poster: 3

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Manufacturing and formation techniques

Keywords: Bi doped GeTe, Thermoelectric, Figure of Merit

Thermoelectric properties of Ge_{1-x}Bi_xTe crystals

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GeTe is a heavily p-type semiconductor, it stabilizes in a non-centrosymmetric rhombohedral structure with an space group R3m at room temperature. Its maximum zT is close to 1.0 near 700 K. Recently, several pseudobinary system have been found to exhibit zT of > 1.75 between 600-800 K [1]. In this work, we report a remarkable thermoelectric figure of merit (zT) of 1.9 in a high-quality Bi doped Ge_{1-x}Bi_xTe crystal with x=0.1, achieved by synergistically optimizing the thermoelectric power factor and thermal conductivity. The substitution of Bi for Ge enables carrier compensates the excess hole in pristine GeTe, and shifts the Fermi level to an eligible energy range. We show that when carrier concentration $p \sim 3.5-5 \times 10^{20} \text{ cm}^{-3}$, the Fermi level intersects with the “pudding mold band” centered at L point that enhances electrical transport properties due to its heavier band mass. Our results also show that the thermoelectric performance is strongly affected by the number of pockets participating in the electrical transport, which is evidenced by the correlation between electrical conductivity and Seebeck coefficient S. Compared to the pristine GeTe, the substitution of Bi for Ge site can drastically bring down the thermal conductivity K, by the minimizing the thermal conductivity of carriers and mass fluctuation alloying effect, and eventually leads to the highly enhanced zT.

Key Words: Bi doped GeTe, Thermoelectric, Figure of Merit

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Wednesday, 21/Aug/2019 6:12pm - 6:24pm

Abstract ID: 474 / FBB: 12

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Advances in Enzymatic and Non-Enzymatic Biosensors

Keywords: Pyrenyl-carbon Nanostructures, Biomarker Sensor, Bio-Electrocatalysis

Robust Pyrenyl Carbon Nanostructures for Biomarker Sensors and Enzyme Electrocatalysis

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The conventional covalent carboxylation (e.g., by acid treatment) and recently evolving noncovalent functionalization of carbon nanostructures have shown promise in the areas of bioelectronics, biosensors, engineering, materials science, fuel cells, and renewable energy. We present here quantitative results of combining covalent and noncovalent pyrenyl carboxylation of carbon nanotubes for developing highly sensitive serum insulin (5800 Da) immunosensor and urine formaldehyde (30 Da) amperometric biosensor with enhanced sensitivity and lower detection limits than the absence of pyrenyl modification. Additional applications to purified enzymes and liver microsomal cytochrome P450s representing novel electrocatalytic platforms for prodrug assays and biosensing will be presented. In view of diagnostic challenges, the molecular size of a biomarker present in complex biofluids inversely affects the detection sensitivity. This is because small molecules do not yield measurable assay signal changes compared to large biomolecules. Hence, developing new electrochemical methodologies for small-molecule biomarkers and stereoselective bio-electrocatalytic applications represents significance in biomedical, pharmaceutical, and in vitro diagnostic applications.

Abstract ID: 475

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: PVA, Nano clay, Packaging, Iraq Ca-bentonite, SEM

Fire resistance, thermal stability and mechanical properties of PVA nanocomposite filled with modified nano Iraqi Ca-bentonite for packaging applications

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The importance of polymers and their composites is increased daily in the domestic and in the industrial fields. Polyvinyl alcohol (PVA) is a polymer which has great attention in recent years because of its characteristic properties. The present work is divided into two main parts. The first part deals with manufacturing nano modified nano clay from Iraq Ca-bentonite (MNCB). The nano modified synthesized nano clay was characterized by XRD FTIR, SEM, AFM, TGA EDS, and XRF. The second part is dealing with synthesizing PVA/MNCB nanocomposite. Different loadings of MNCB were added to PVA (0%, 5 %, 10% and 15% of PVA weight). The nanocomposites samples were investigated and characterized by different techniques to assess their performance. The mechanical test was tensile. Thermal stability was tested using DSC and TGA. While the crystallinity of polymer samples was calculated using XRD and DSC tests. The fire resistance properties of synthesized samples were assessed via Limited oxygen index (L.O.I), U-94 protocol tests. Besides, FTIR test was done to investigate bonding structure and the morphology of nanocomposites samples was tested via SEM test. . The results of the work showed the positive role of MNCB on the properties of PVA polymer. The mechanical properties, thermal stability were improved. The fire retardancy assessment showed that the importance of using MNCB as a new green fire retardant for PVA. The whole results of work assured on the success of synthesis of nano-clay from Ca-Bentonite. In addition, the results reflect the benefits of using this filler in improving the different properties of PVA/MNCB nanocomposite.

Thursday, 22/Aug/2019 12:36pm - 12:48pm

Abstract ID: 476 / FTF: 9

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Nanostructured and Architecturally Designed Coatings, Smart Surfaces

Keywords: nanostructures, polysiloxane, silicone nanofilaments, germanium oxide

The DAGS-Chemistry: Droplet Assisted Growth and Shaping for Synthesis of Polymeric Nano- And Microstructures

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The synthesis of nano and microstructures is an emerging field in chemistry and materials science. Such structures and structured films can be synthesized from a large variety of materials, for example metals, semi-metals, or polymeric substances. Usually, these particles exhibit a comparable simple shape, for some a high temperature is required and for many (except polymers) of them no covalent bonds are formed during formation /1/.

Some years ago, we have presented the synthesis of silicone nanofilaments in particular for coatings delivering superhydrophobic, superoleophobic, or superamphiphobic surface properties (fig. 1) /2, 3/. Also, nano- and microstructures different from filaments have been synthesized in a reproducible manner /4/.

Recently, we have shown the reaction mechanism underlying this unusual one-dimensional growths /5/. Based on this new scheme we are able to synthesize silicone nano- and microparticles of different shapes depending on the reaction conditions. Some of these structures exhibit a shape complexity which goes clearly beyond wires and filaments.

The mechanism of this synthesis is applicable not only to silicone structures but also to other chemical compounds, for example germanium oxide and aluminum oxide nanofilaments.

In this presentation, we will give an overview about this novel synthesis scheme which we call “Droplet Assisted Growth and Shaping” (DAGS) approach. Applying appropriate reaction conditions allows for the directed growth of nano- and microstructures of complex shape. We believe that this reaction scheme is very promising in chemical synthesis and material science, since it enables us to form complex nano and microstructures from polymeric materials at room temperature in aqueous medium.

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Thursday, 22/Aug/2019 10:00am - 10:12am

Abstract ID: 477 / FLNM: 11

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Fundamental investigations on low-dimensional nanomaterials and their functional structures properties

Keywords: Flexoelectricity, Graphene, Nanosheet, Molecular dynamics

Flexoelectric effect of low-dimensional graphene nanosheets

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Flexoelectricity is a universal effect existing in all dielectrics even with symmetric structures. Unlike piezoelectricity, flexoelectricity is strongly size dependent. This is why the flexoelectric effect is understudied in macro scale. We choose graphene nanosheets as our research object, because large strain gradients can be obtained more easily in low-dimensional materials. We study the symmetry properties of flexoelectricity in hexagonal crystals and find out there are in total seven independent constants. Molecular dynamics simulations using LAMMPS computational package are conducted to add strain gradients in few-layers graphene nanosheets. Linear response between polarization and strain gradient is demonstrated. The simulation results are used to calculate the flexoelectric coefficient of graphene. Our research paves the way for understanding flexoelectricity theoretically and exploration of flexoelectric energy harvesters.

Abstract ID: 478 / Poster: 4

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Advances in Enzymatic and Non-Enzymatic Biosensors

Keywords: Electrochemical aptasensor; Magnetic biocomposites; Pb²⁺-dependent DNAzyme; Thrombin

A label-free electrochemical aptasensor based on magnetic biocomposites with Pb²⁺-dependent DNAzyme for the detection of thrombin

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Thrombin can accelerate the occurrence of various diseases such as venous thromboembolism, nephropathy and central nervous system diseases. Thrombin, an important biomarker, is used to assist the early diagnosis and treatment of clinical diseases. However, the current clinical examination is mainly four blood coagulation indexes, lacking direct detection methods for thrombin. In this study, a label-free electrochemical aptasensor for the detection of thrombin based on magnetic biocomposites and Pb²⁺-dependent DNAzyme was designed and constructed. Under the action of the aptamer element and the magnetic composite nanomaterial, the recognition and separation process was realized. The electrochemical signal amplification is realized under the action of Pb²⁺-dependent DNAzyme. Electrochemical signal was recorded by electro-static interaction between methylene blue (MB) and DNA. The magnetic biocomposites were adsorbed by magnetic field induced self-assembly on the surface of magnetic glassy carbon electrode. Thus, the thrombin detection could be recorded by monitoring the electrochemical signal of MB. The method realizes the highly sensitive and high-selective detection of thrombin by the electrochemical aptasensor, and is successfully used for the detection of clinical samples, and provides a powerful means for clinical diagnosis and treatment.

Thursday, 22/Aug/2019 10:18am - 10:30am

Abstract ID: 479 / FCM-2: 12

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Porous and cellular materials

Keywords: heat storage, porous metal structure, zeolite, heat accumulator, heat transfer

The effect of Al-based cellular structure on the thermal performance of the zeolite based hybrid heat accumulator

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The designed heat accumulator consists from the 12 blocks of the metal foam structures of 10 PPI cast by the means of investment casting technique from Al-Si alloy (EN AC-44200) immersed in the zeolite 4A (3-5 mm, laboratory grade), that was provided by the United Quantum Factory Ltd., Poland. The porous metal structure characterized by the relatively large coefficient of thermal conductivity effects on the rapid transport of the heat energy from the heat source to the heat accumulator.

In the industrial practice the heat accumulator is charged from the solar sources and in order to simulate the conditions of solar heating, the heating stage was being simulated by the use of the two outdoor halogen reflectors of 400 W each. Set point of the heat source controller was established at 300°C. The loading phase of the accumulator was evaluated as the raise of the temperature as the function of time by the type K thermocouples located on the bottom, in the middle and on the top of the heat accumulator. Data acquisition was performed with the use of the computer and the National Instruments DAQ system. Multiple long-term cycles of charging and discharging of such accumulator, with and without metallic porous inserts improving the thermal conductivity and heat transfer area, were conducted and subsequently analyzed. The effect of the porous cellular structure on the rate of charging and discharging of the heat accumulator was established and further discussed.

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Abstract ID: 480

Symposium 2: Functional Composite Materials (FCM)

Invited Talk

Topics: Electro-thermal properties of composite materials

Keywords: Iron based superconductors, thermal conductivity, resistivity, Seebeck coefficient

Measurement and analysis of thermoelectric properties of FeSe superconductor

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Thermoelectric properties such as thermal conductivity (κ), Seebeck coefficient (S) and electrical resistivity (ρ) of the FeSe superconductor were measured and analyzed. The samples were synthesized through a solid state reaction route via vacuum encapsulation and characterized by X-ray diffraction studies. Seebeck coefficient S(T) exhibits an anomalous temperature dependence and shows a crossover of sign at around 190 K, which is an artifact of coexistence of electron and hole bands. Along with carrier diffusive Seebeck coefficient $S_{diff}(T)$, phonon drag contribution $S_{phdrag}(T)$ can successfully explain the experimental results. The measured thermal conductivity, $\kappa(T)$ develops a phonon peak at around 80 K, which is an artifact of various phonon scattering mechanisms. Along with phonon thermal conductivity κ_{ph} , the carrier contribution κ_c is also important, particularly at higher temperatures around room temperature. Electrical resistivity of FeSe shows superconducting transition at temperature T_C around 10 K and shows metallic temperature dependence above T_C which is explained using the Bloch-Grüneisen (BG) function of temperature dependence resistivity.

Abstract ID: 481

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Polymeric composites

Keywords: pectin, PLGA, hydrogel, cross-linked, biodegradable

Fabrication of Cross-linked Pectin Hydrogel for Control Drug Delivery Application

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The present study was aimed to design and develop biodegradable pectin hydrogel blend with stable agent poly ethylene glycol (PEG) physical cross-linked with the Tetraethyl orthosilicate (TEOS). Pectin, due to its ideal behavior as drug vehicle with different drugs loading, chemistry binding or encapsulation, its biodegradable hydrogel loaded with different chemotherapeutic drugs grasping the attention for cancer treatments. Anti-cancer drugs have reduced water solubility and poor control release to targeted areas, to enhance the targeted delivery of drug novel pectin based cross-linked hydrogel was developed with help of two series i.e., series 1 with different concentration of TEOS (1 M, 7.5 M, 0.50 M and 0.25 M) and series 2 with different molecular weight of PEG (300, 600, 1500 and 6000). Fabricated novel biocompatible pectin hydrogel was structurally and morphologically analyzed with Fourier Transform Infrared Spectroscopy, Thermal gravimetric Analysis, X-Ray Diffraction, Scanning Electron Microscopy and swelling behavior in water and ionic solutions. Results showed that TEOS with 0.75 M concentration and PEG 6000 in pectin hydrogel resulted in hydrogel with good swelling ratio in water and ionic solution. Anti-cancer drug Cisplatin was loaded in cross-linked pectin hydrogel to study control drug release in simulated gastric fluid (SGF) and simulated intestinal fluid (SIF). The in-vitro release of drug studied by UV- visible spectrophotometer at 290 nm in SGF was found to 9.32 % in 2 hours and in SIF it was 86.67 % in 3 hours. Current development and control drug release of cross-linked Pectin-PEG hydrogel demonstrated to it as a promising drug vehicle for cancer treatment. It is also proposed that FDA approved Poly lactide co glycolide (PLGA) with stable agent PEG loaded in pectin hydrogel for anti-cancer nano drug delivery.

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Thursday, 22/Aug/2019 2:27pm - 2:39pm

Abstract ID: 482 / FLNM-3: 3

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nanomaterials for Energy and Environmental Applications

Keywords: Photocatalysis, Water splitting, Hydrogen generation, Nanoparticles, Heterostructures, Solar to fuel conversion

Sculpting Photocatalysts on the Nano Scale

Lilac Amirav

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The solar-driven photocatalytic splitting of water into hydrogen and oxygen is a potential source of clean and renewable fuels. However, four decades of global research have proven this multi-step reaction to be highly challenging. The design of effective artificial photo-catalytic systems will depend on our ability to correlate the photocatalyst structure, composition, and morphology with its activity.

I will present our strategies, and most recent results, in taking photocatalyst production to new and unexplored frontiers. I will focus on unique design of innovative nano scale particles, which harness nano phenomena for improved activity, and methodologies for the construction of sophisticated heterostructures. I will share our design rules and accumulated insights, which enabled us to obtain a perfect 100% photon-to-hydrogen production efficiency, under visible light illumination, for the photocatalytic water splitting reduction half reaction. Finally, I will describe our future designs of systems capable of overall water splitting and genuine solar-to-fuel energy conversion.

Abstract ID: 483

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Artificial photosynthesis

Keywords: Photocatalysis, Water splitting, Hydrogen generation, Nanoparticles, Heterostructures, Solar to fuel conversion

Sculpting Photocatalysts on the Nano Scale

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I will present our strategies, and most recent results, in taking photocatalyst production to new and unexplored frontiers. I will focus on unique design of innovative nano scale particles, which harness nano phenomena for improved activity, and methodologies for the construction of sophisticated heterostructures. I will share our design rules and accumulated insights, which enabled us to obtain a perfect 100% photon-to-hydrogen production efficiency, under visible light illumination, for the photocatalytic water splitting reduction half reaction. Finally, I will describe our future designs of systems capable of overall water splitting and genuine solar-to-fuel energy conversion.

Abstract ID: 484

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Fuel Cells

Keywords: Oxygen Reduction Reaction, Electrocatalysis, d-band center

**Relationship between ORR Activity and d-band Center of Pt and Pt-based Alloy
Nanoparticle Deposited on Metal Oxide Support Materials**

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Platinum nanoparticles (Pt NPs) have been selectively anchored by photodeposition on titanium oxide (TiO₂) matrix which is formed by hydrolysis of titanium isopropoxide on cup-stacked carbon nanotubes (CSCNT) in isopropanol, producing the composite Pt catalyst useful for oxygen reduction reaction (ORR) in acidic media, i.e., Pt NPs/TiO₂/CSCNT. Using scanning transmission electron microscopy (STEM) with a high-angle annular-dark-field (HAADF) detector it has been clarified that Pt NPs are sunk into the TiO₂ moieties and have the unique polyhedral shape surrounded mainly by the Pt (1 1 1) and Pt (1 0 0) facets. X-ray photoelectron spectroscopy (XPS) allowed us to confirm changes in electronic properties of both Pt NPs and TiO₂ support, induced by the so-called strong metal-support interactions (SMSI) and the significantly increased ORR activity was attained in 0.1 M HClO₄, compared with the Pt NPs deposited on CB (Vulcan carbon) and CSCNT. The surface structure of the Pt NPs was characterized by transmission electron microscopy (TEM), indicating the improved durability of the Pt NPs deposited on the TiO₂/CSCNT, i.e., the only slight increase in the particle size after the durability test (typically 2000 times' potential cycling at 10 mV s⁻¹ in the potential ranges of 0.05 to 1.1 V and 1.0 to 1.5 V vs. RHE in 0.1 M HClO₄). The results obtained demonstrate that the anchoring of Pt NPs on the TiO₂ support material deposited on CSCNT is an effective way to enhance the ORR activity of Pt NPs by the SMSI as well as to prohibit Pt NPs from aggregating, i.e., the degradation of the ORR activity of Pt NPs.

Abstract ID: 485

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

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

Keywords: ferrofluids, transformer, nanoparticles, magnitute

Ferrofluid for transformers: is obtained by modification of mineral oil with magnetite nanoparticles Fe₃O₄

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Ferrofluids based on insulating liquids are intensively studied as a potential substitute of liquid dielectric in high voltage technologies. In this work we focus on the experimental investigation of flow and thermal transport characteristics of a ferrofluid based on transformer oil (Mogul) and iron oxide nanoparticles.

Abstract ID: 486

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Photonic and optoelectronic device applications of low dimensional, nano and 2D materials

Keywords: 2D layered materials, 2D non-layered materials, Van der Waals epitaxial growth, electronic and optoelectronic applications

Two-Dimensional Metal Chalcogenide Semiconductors: Design, Synthesis and Applications

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While scaling the dimension(s) of semiconductors down to nanoscale, novel properties, such as ultrahigh specific surfaces and strong electrostatic tunability, will show out. Among the various low dimensional structures, two-dimensional (2D) semiconductors may lead the next generation of electronics and optoelectronics due to their compatibility with traditional micro-fabrication techniques and flexible substrates. Up to now, both layered and non-layered materials have been demonstrated to present in 2D geometry. As for the former, even though big breakthroughs, especially on transition metal dichalcogenides (TMDCs), have been made, more systematical and deeper studies are needed. In addition, inspired by the success of 2D layered materials and the fact that many materials with significant functions have non-layered crystal structures, 2D non-layered materials have attracted increasing attentions. Based on above challenges and motivations, our research focuses on the design, synthesis and applications of low dimensional metal chalcogenides semiconductors. In this talk, I will present our recent progress on the following two aspects:

(1) 2D layered metal chalcogenide semiconductors: controllable synthesis, properties, electronic and optoelectronic applications. [1, 3-5, 7, 10]

(2) Van der Waals epitaxial growth, electronic and optoelectronic properties of 2D non-layered materials, such as CdTe, PbS and $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ nanosheets. [2, 6, 8, 9]

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Thursday, 22/Aug/2019 9:54am - 10:06am

Abstract ID: 487 / FCM-2: 10

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Carbon and metal oxide based composite materials

Keywords: pyrolysis, magnetic, core-shell, electromagnetic wave absorption, composite

One-pot synthesis of a lightweight effective electromagnetic wave absorber, Fe/Fe₃O₄@C, via in situ carbonization of Fe₃O₄-lignin framework

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Along with the quick development of electronic devices and communication technology, it is widely accepted that we need an ideal electromagnetic wave (EMW) absorber to solve the electromagnetic interference (EMI) irradiation pollution. One of this kind of absorbers are composites of carbon and ferromagnetic metal with special morphologies and varied interfaces, being desirable to obtain excellent electromagnetic impedance matching. However, there are merely researches on the synthesis of such absorbers, and the corresponding analysis of the EMW energy loss mechanism remains great challenges. Here, we successfully synthesized graphite/Fe₃O₄/Fe composites (GFF) by carbonizing Fe₃O₄-lignin frameworks which were prepared through a two-step carbodiimide coupling protocol. The in-depth investigation confirmed the composites were Fe/Fe₃O₄ core/shell particles inlaid in graphite-like matrix. The obtained GFF displayed excellent EMW absorbing performance with a minimum value of -47.11 dB and a wide response bandwidth (reflection loss of less than -10 dB) of 5.64 GHz. This excellent performance is attributed to the optimal dielectric loss caused by the dipolar and multiple interfacial polarization, migration and hopping of electrons in the graphite-like carbonized matrix, and to the optimal magnetic loss from natural resonance and exchange resonance of the inlaid Fe/Fe₃O₄ core-shell nanoparticles in the matrix. Besides, the carbon matrix with a certain graphite degree effectively regulates the complex permittivity and permeability to ensure the impedance matching characteristic as well as enhance the attenuation ability through the multiple reflections and scatterings among the inlaid Fe/Fe₃O₄ core-shell nanoparticles. The obtained GFF has been proved to be a promising candidate for practical application to EMW absorption by the effective usage of the pulping and papermaking industry by-product, lignin.

Abstract ID: 488

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Imaging

Keywords: DNA nanoassembly, proximity hybridization, HER2 dimerization, fluorescent imaging

Colocalization-triggered DNA nanoassembly for facile and amplified imaging of HER2 dimerization on cancer cell surface in tissue samples

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Convenient and sensitive detection of human epidermal growth factor receptor 2 (HER2) dimerization is highly desirable for molecule subtyping and guiding personalized HER2 targeted therapy of breast cancer. Herein, we proposed an aptamer colocalization-triggered DNA nanoassembly (CtDNA) strategy for simple and amplified imaging of HER2 dimerization on cancer cell surface. Two aptamer probes simultaneously localize on the dimeric HER2 proteins, induce proximity hybridization, and further initiate hairpin-free nonlinear HCR, forming DNA dendritic nanostructure for in-situ signal amplification and fluorescent imaging of HER2 dimers. This CtDNA strategy was used to identify HER2 homo- and hetero- dimers on different breast cancer cell lines via general fluorescence microscopy with high specificity and sensitivity. Furthermore, this approach has been successfully applied to image and quantitatively evaluate HER2 homodimers in real breast cancer tissue specimens, proving its remarkable accuracy and practicality for real sample analysis. Therefore, the proposed CtDNA strategy would become a powerful and pragmatic toolbox to conveniently and sensitively detect receptor dimerization in clinical samples for improving clinical research, cancer diagnostics and personalization treatment.

Abstract ID: 489

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Nanogenerators and self-powered nanosystems

Keywords: Vibration Energy Harvester, Fe-Ga Alloy Film, Instantaneous Vibration Energy, Continuous Resonant

A New Continuous Resonant Vibration Harvester Using Fe-Ga Alloy Film For Harvesting Instantaneous Vibration Energy

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Vibration energy harvesting technology has been a research subject of growing interest over the past few years. And it may be a new way to overcome the unsatisfactory battery issue in low-power electronic devices, such as wireless sensors. Different mechanical-to-electrical energy conversion methods have been exploited on the basis of different functional materials, such as piezoelectric and magnetostrictive methods. Compared with piezoelectric materials and traditional Terfenal-D alloy, Fe-Ga alloy offers excellent properties for surviving in tough ambient vibration conditions, including excellent robustness, higher energy conversion efficiency, and higher flexibility, etc. In this study, we propose a new instantaneous frequency converted to high frequency- vibration energy harvester using a Fe-Ga alloy film as the transducing element to harvest low-frequency vibration energy. The harvester consists two parts: a frequency conversion mechanism and a vibration harvesting mechanism. To effectively harness energy in instantaneous low-frequency conditions, a frequency conversion mechanism that succeeds in converting instantaneous impact vibration in low-frequency up to the system's continuous resonance in higher-frequency is developed. The design of the vibration energy harvester is based on the coupling characteristics of magnetostrictive inverse effect and Faraday electromagnetic induction. The vibration harvesting mechanism consists of a cantilever beam consisting of a Fe-Ga alloy film with two substrates and a pickup coil. Fe-Ga alloy film has magnetostrictive inverse effect during vibration and the internal magnetization state will change. The cantilever beam is surrounded by a pickup coil and voltage is induced due to the Faraday electromagnetic induction. A comprehensive energy harvesting model is built and solved to analyze the mechanical-magnetic-electrical coupling system. A prototype is fabricated with a Fe-Ga alloy film of 0.5 × 10 × 50mm³ and, instantaneous impact vibration, it generates 6 mW power. The influence law of excitation and structure conditions and substrate's material on output electrical power are investigated in comprehensive experiments.

Abstract ID: 490

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Nanogenerators and self-powered nanosystems

Keywords: Energy harvesting, Triboelectric effect, energy-loss

Sustainable energy harvesting technology based on triboelectric nanogenerators and loss-energy harvesting system

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As the energy crisis and global warming are emerging as major issues, the development of renewable and green energy based on alternative energy resources such as solar, wind, hydrogen or geothermal sources, has attracted considerable interest. The energy harvesting technologies based on these natural resources have been well established, and their use has gradually increased. Yet there are still many forms of energy sources in our living environment, which are not being utilized. Further, owing to increasing energy demands, significant energy-related issues remain to be solved. Thus, we need to continue the efforts to develop innovative energy harvesting technology to overcome energy issues. Here, we introduce two strategies for a sustainable energy harvesting method: 1) Mechanical energy harvester based on triboelectric effect and 2) Loss-energy harvesting system.

Abstract ID: 491

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Applications of Biopolymer for Drug Delivery

Keywords: cancer therapy, drug nano-carrier, responsive core/shell nanoparticles

Smart superparamagnetic nano-carrier for cancer therapy

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Grafting functional biocompatible thermo-responsive copolymers at the surface of superparamagnetic nanoparticles (NPs) is a promising route to develop new targeting nano-carriers for cancer therapy. In this work, we report on the development and the characterization of superparamagnetic and thermo-responsive core/shell NPs which were used as a drug delivery based system. These NPs were obtained by the growth via controlled living polymerization of co-polymers based on 2-(2-methoxy) ethyl methacrylate (MEO2MA) and oligo (ethylene glycol) methacrylate (OEGMA) moieties leading to P(MEO2MA_x-OEGMA100-X) (the ratio of the both monomers were varied to tune the LCST)^{1–5}. We demonstrate that the NPs are able to load and release a model drug, i. e. doxorubicine (DOX) with an associated DOX loading capacity of 93%, markedly higher than the current nanocarrier performances. Those new systems exhibit also hyperthermia properties. The cytotoxicity results showed that the core/shell NPs exhibit limited cytotoxicity up to concentration of 12 mg.mL⁻¹ towards SKOV3 human ovarian cancer lines. Upon DOX release from DOX-loaded NPs, the NPs are much more cytotoxic towards those cells than free DOX. Moreover, when folic acid (FA) was anchored at the periphery of these NPs³, an enhancement of the selective binding and of the delivery of the drug to the targeted cells (SKOV 3) was demonstrated.

This study offers a promising route to improve the current available drug nanocarrier for cancer therapy combining in one nano-object hyperthermia and chemotherapy.

Key Words: cancer therapy, drug nano-carrier, responsive core/shell nanoparticles

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Abstract ID: 492

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Sol-gel and LB technology

Keywords: recycled polystyrene, sol-gel, hybrids

DEVELOPMENT OF HYBRID FILMS BY RECYCLED POLYSTYRENE

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Current challenges for the reuse of various polymers, hybrids materials and in the study of their properties are considered. This work shows an alternative to reuse Polystyrene of beverage containers, through to preparing hybrids consisting silica nanoparticles embedded in polystyrene recycled matrix. The polymer matrix (polystyrene recycled and not recycled) was in situ functionalized with the purpose to modify the surface during the sol-gel process. Polystyrene matrix functionalized was used to influence the morphological and properties such as, optical, antifog, degradation by UV irradiation, thermal stability and mechanical properties. These hybrid materials were prepared with polystyrene recycled (SiO₂/PSR) and polystyrene recycled functionalized (SiO₂/PSR-F) and compared with the commercial polystyrene (PS) hybrids. These materials were used as surface coatings on glass. The cytotoxicity of the PSR films without substrate was evaluated, showing viability to be used as protective films on glass substrates, this is of high relevance because they do not present a health risk. The hydrophobicity of the coatings was determinate by contact angle measurement. The degradation of the hybrid coating was determined before and after exposure irradiation UV at 364nm by FT-IR and UV-Vis spectrosopes. The hybrids were characterized by Infrared technique and evaluated their mechanical properties.

Abstract ID: 493

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Additive manufacturing Applications

Keywords: Rapid tooling, Ultra-large, Injection mold, Conformal cooling channels

A cost-effective approach using recycled materials for rapid manufacturing ultra-large injection mold with conformal cooling channels

Chil-Chyuan Kuo, Yi-Jun Zhu, Ying-Zhi Wu, Zheng-Yan You

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Production cost is an important issue for manufacturing a die or mold in the new product development phase, especially for an ultra-large die or mold. In this study, a cost-effective approach to manufacture an ultra-large injection mold with conformal cooling channels was proposed. Recycled materials were used to manufacture an ultra-large injection mold. It was found that an ultra-large injection mold with conformal cooling channels can be fabricated swiftly and effectively through an intermediary mold. The production costs savings about 83.4% can be obtained. An obvious reduction in cooling time of about 94.7% can be obtained when a wax injection mold with conformal cooling channels compared to that without cooling channels. Roundness of the conformal cooling channel in the mold fabricated by rapid tooling technology (RTT) is obviously superior to that fabricated by metal additive manufacturing (MAM) technology. In addition, the surface roughness of the molds fabricated by RTT is superior to that for the mold fabricated by MAM technology. In addition, the surface quality of cooling channel wall of the mold fabricated by RTT is superior to that for the mold fabricated by SLS technology. It is interesting to note that the approach proposed in this study meet the objectives of green manufacturing and provides the greatest application potential in the precision machinery because of the production cost reduction increases with increasing the sizes of the intermediary mold.

Thursday, 22/Aug/2019 9:12am - 9:24am

Abstract ID: 494 / FESC: 7

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Advances in electrolyte and electrolyte additives for energy storage devices

Keywords: Graphene, Polyaniline nanofiber, Hybrids, Supercapacitor

Layer-by-layer fabrication of multilayer hybrids composed of graphene/polyaniline nanofiber for high-energy electrode materials for supercapacitors

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Polyaniline was one of the conducting polymers widely used in supercapacitors. However, due to its low conductivity and aggregation, the specific capacitance of polyaniline material prepared is much lower than its theoretical specific capacitance. In this work, multilayer hybrids composed of pristine graphene and polyaniline nanofiber were prepared via vacuum filtration to assemble high-performance supercapacitor. The polyaniline nanofiber distributed uniformly between graphene layers. After adding graphene, the specific capacitance of the hybrids electrode in the three-electrode system was improved from 379 F/g to 565 F/g at a current density of 0.1 A/g. The crosslinking network of polyaniline nanofiber provided more charge transmission pathways, and fast charge-transfer speed of electrons to the pristine graphene and the pristine graphene intercalated into polyaniline nanofiber layers improved the electrical conductivity as well as shorten the charge transmission pathways of electrons. The hybrid is expected to have potential applications in supercapacitor electrode.

Abstract ID: 495

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Metal organic framework, gas separation

Metal–Organic Framework with Trifluoromethyl Groups for Selective C₂H₂ and CO₂ Adsorption

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These two decades have witnessed the rapid development of metal-organic frameworks (MOFs) due to their unique structures and various potential applications, e.g. strategic gases storage/separation, and catalysis. Exploring mixed ligands techniques to construct MOFs is of high interests for gas separation developments. We demonstrate a simple strategy to build nets derived from the net of the primitive cubic lattice (pcu) of microporous SIFSIX-type MOF. Reaction of CuSiF₆·xH₂O and 1,4-bis(4-pyridyl)-2-trifluoromethylbenzene (bpb-CF₃) through liquid diffusion produces allow to form new materials of [Cu(bpb-CF₃)₂(SiF₆)] (UTSA-121) containing functional trifluoromethyl groups. Mixed ligands (SiF₆²⁻ and bpb-CF₃) tactics are indicated as a source of MOF versatility and are critical to the design process and thus to rationally tune the micropores to size exclusively trap C₂H₂ and CO₂ over CH₄ under ambient conditions.

Abstract ID: 496

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Enzymes and Biocatalysts

Keywords: Haloalkaliphilic bacteria, metagenomics, gene cloning, recombinant enzymes, protease diversity

Diversity, expression and characteristics of extracellular proteases of Haloalkaliphilic bacteria from the Coastal Gujarat, India

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Over the years, we have studied distribution, diversity and enzymatic characteristics of haloalkaliphilic bacteria and actinomycetes. In this presentation, we describe the diversity of protease genes, its expression and enzymatic characteristics. The genetic diversity of the protease genes was studied by the PCR amplification using variety of primers followed by sequencing and analysis of the ORF's. The widely distributed extracellular proteases in these organisms represent unique common properties of salt dependent temperature profile, resistance against chemical denaturation and catalysis under multitude of the extremity. The molecular cloning, sequence analyses and characteristics of the recombinant proteases of the cultivable and non-cultivable bacteria reflect molecular and enzymatic diversity.

Wednesday, 21/Aug/2019 4:12pm - 4:24pm

Abstract ID: 497 / FBB: 2

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Advances in Enzymatic and Non-Enzymatic Biosensors

Keywords: sensors, potassium ion sensors, synthesis

Fluorescent potassium ion sensors

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Potassium ions which make up about 0.4% of the mass in the human body and are the most abundant intracellular cation, play diverse roles in biological processes including muscle contraction, heartbeat, nerve transmissions, and kidney functions. Abnormal K⁺ fluctuations are early indicators of diseases such as alcoholism, anorexia, bulimia, heart disease, diabetes, AIDS, and cancer. Therefore the detection of K⁺ in physiological environment is of great significance. One of the earliest and best-known intracellular fluorescent K⁺ probes is potassium-binding benzofuran isophthalate (PBFI), which uses a diaz-18-crown-6 as a ligand and a benzofuran derivative as the fluorophore. Unfortunately PBFI, suffers poor selectivity for potassium ions with respect to sodium ions (Na⁺).

Herein, we will describe our results for developing highly selective potassium ion sensors. We used triazacryptand (TAC) as a high selective potassium ion ligand and various fluorophores for preparing highly selective potassium molecular and planar polymeric probes. We constructed a potassium ion sensor using a 2-dicyanomethylene-3-cyano-4,5,5-trimethyl-2,5-dihydrofuran (TCF) as a strong electron withdrawing group and the TAC as the electron donating group for the first intracellular potassium ion sensor. Later we incorporated a triphenylphosphonium (TPP) unit into a BODIPY fluorophore with TAC as the ligand for the first mitochondrial targeting potassium ion probe. These two molecular probes show high selectivity for potassium ions and capable for monitoring intracellular potassium fluxes. Especially the probe with TPP moiety showed high co-localization efficiency for mitochondria. We also prepared a polymerizable potassium ion probe using naphthalimide as the fluorophore for generation of planar thin film-based potassium ion sensors. These polymeric sensors showed potassium ion dynamic response ranges from 1 to 20 mM, indicating its suitability for extracellular sensing. This sensor also has a minimum influence by pH from 6 to 8, showing its suitability for biostudies. We tested whether this sensor can be used to monitor extracellular potassium ion concentration changes. We used lysozyme to kill bacteria (*E. Coli* and *B. Subtilis*) to release their cellular potassium ions to the media to enable us to monitor potassium concentration changes in real time. Results showed that potassium ion concentration is higher with higher cell densities. We also found the difference among the two species of cells. *E. coli* release potassium ions much slower than that *Subtilis* did. Thus in this presentation, we will give detailed results about our potassium ion sensors.

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Abstract ID: 498

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Nanomaterials for Sensors, Flexible Electronics and Nanocomposites

Keywords: Green Printing, Nano, Functional Patterns, Devices

Green Printing Technology for Manufacturing Functional Devices

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Based on the droplet drying process on the surfaces of different wettability, controllable nanoparticles assembling and patterning could be achieved, through controlling the movement of vapor-liquid-solid three phase contact lines. Highly precise self-assembly of nanomaterials in the ink droplets along the vapor-solid-liquid three phase contact lines could be accurately achieved. [1] Significantly, the basic units (dot, line, plane and stereo structures) via the printing technology can be precisely controlled. [2] We achieved the silver nanoparticles assembled conductive patterns with one nanoparticle (12 ± 3 nm) resolution.[3] Our further work on assemble metal nanomaterials or graphene via feasible printed process, patterned the various linear or curves 1D/2D morphologies and optimal interconnects on diverse substrates.[4] The desirable conductive patterns contribute the remarkable application on sensitive electrical skin[4a], transparent touch screen[4b,c], multi-layer circuits[4d], ultra-integrated complex circuits[4e] and soft actuators[4f]. This achievement on printed electronics are derived and benefited from the fundamental researches on solid/liquid interfacial wettability manipulation, morphology control of dried ink droplets, as well as functional nanomaterial fabrication, which construct the theoretical and technical system, Green Printing Technology.

Figure Green printing technology based on droplet manipulation.

Key Words: Green Printing, Nano, Functional Patterns, Devices

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Abstract ID: 499

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Electrochemical Supercapacitors

Keywords: BiPO₄, Nanostructures, Energy Storage

Microwave-Assisted Synthesis of BiPO₄ Nanostructures for Supercapacitor Applications

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Microwave-Assisted Synthesis of BiPO₄ Nanostructures for Supercapacitor Applications

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With the increasing demands for energy problem, there is a need for society to develop some novel technological systems applicable to conversion of alternative energy sources and fabrication of new energy storage devices. Among the various energy storage devices, supercapacitor has attracted significant attention due to their high power density, long cycle life, high efficiency, eco-friendly and safe compared with batteries. They are utilized in numerous applications such as consumer electronics, hybrid vehicles, memory backup system etc. The performance of supercapacitors is intimately related to the electrode materials. The development of new electrode materials that are low-cost and environmentally friendly have been progressing rapidly with the advancement of materials, design strategies, synthesis techniques, and characterization methodologies. Transition metal oxides such as ZnO, CuO, Fe₂O₃, RuO₂, MnO₂, V₂O₅ and metal phosphates such as BiPO₄ are the most popular electrode materials for supercapacitors. In the present work, we reported the effects of time and temperature on structural, optical and electrochemical properties of BiPO₄ nanostructures synthesized via microwave assisted technique. The structure and morphology of BiPO₄ were systematically characterized by X-ray diffraction (XRD) and Field emission scanning electron microscopy (FESEM) studies. The electrochemical studies were recorded using an electrochemical system.

Key Words: BiPO₄, Nanostructures, Energy Storage

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Abstract ID: 500

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Magnetic Materials

Keywords: Magnetic nanoparticles; Atomic layer deposition, Removal templates.

ZnO Ultra-Thin Films Growth on Magneto-Controllable Core-Shell Nanoparticles Encapsulated With a Removable SiO₂ Template

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Nowadays, a research area of great interest in nanotechnology is the development of nanoparticles for different applications. This work focus in core-shell nanostructures synthesis based on Co_{0.25}Zn_{0.75}Fe₂O₄ ferrite nanoparticles with superparamagnetic behavior [1] via chemical co-precipitation method from aqueous salt solutions in alkaline medium and coated with a silica shell (SiO₂), through the sol-gel method as removable template. ZnO ultrathin layer was growth over SiO₂ template via atomic layer deposition technique (ALD). After coating the template with ZnO, it was removed via chemical method in order to obtain a functional material with interesting properties that can be applied in photocatalysis, magnetic separation and drug transport. Nanostructures were characterized by XRD, VSM and TEM in order to study the structural, magnetic behavior, removable template morphology, particles size and ZnO coat thickness. TEM measures for zinc-cobalt ferrites coated with silicon oxide allows to observe nanoparticles with a diameter size distribution between 7 and 11 nm and ZnO layer thickness with approximately 30 nm. Magnetic measures from M vs H loops, indicate a tendency superparamagnetic behavior which is a good indicator of the high magnetization capacity. X-rays diffraction pattern allowed confirm spinel structure formation, features this kind of ferrite. This results opens the possibility to use this functional materials in different nanotechnology fields.

Acknowledgment: This work was partially supported by Dirección General de Asuntos del Personal Académico DGAPAUNAM, through research projects: Ciencia Básica A1-S-21323, PAPIIT IN105114, IN112117, IN107715, PAPIME 2017 project PE101317 and FORDECYT - CONACYT 272894 project.

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Abstract ID: 501

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Thin films for optoelectronics, nanoelectronics and spintronics

Keywords: MOS capacitors; electrical and optical properties; atomic layer deposition, impedance spectroscopy.

Electrical and Optical Properties in Ultrathin Capacitors Base on Al₂O₃ – Y₂O₃ Growth Via Atomic Layer Deposition

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This work focuses on the study of the electrical and optical properties in ultrathin capacitors based on Al₂O₃ – Y₂O₃ bilayers. A set of 10 samples with a total thickness of about 10 nm were grown by means of thermal atomic layer deposition (ALD) on n-type (100) silicon substrates from Trimethylaluminum (TMA), Tris (methylcyclopentadienyl) yttrium ((MeCp₃)₃Y) and water as co-reactants. Thickness and optical parameters were studied via spectroscopic ellipsometry in order to obtain information about the refractive index and dielectric constant behavior. Ellipsometric data revealed an increase of the refractive index when the Y₂O₃ layer thickness varies between 1 and 9 nm. Electrical characterization from Capacitance-Voltage (C-V), Current-Voltage (I-V), capacitance - frequency (c-f), impedance - frequency (z-f) measurements was carried out in order to evaluate the potential of the MOS ultrathin capacitors for micro and nano electronic applications. Results demonstrate that electrical and optical parameters can be modulated by varying the Y₂O₃ layer thickness.

Keywords: MOS capacitors; electrical and optical properties; atomic layer deposition, impedance spectroscopy.

Acknowledgment: This work was partially supported by Dirección General de Asuntos del Personal Académico DGAPAUNAM, through research projects: PAPIIT IN112117, IN110018, IA101018, PAPIME PE101317, PE100318 and FORDECYT - CONACYT 272894 project.

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Abstract ID: 502

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Optical, Optoelectronic and Dielectric Coatings

Keywords: Optical coating; multilayers stacks; dielectric mirror atomic layer deposition.

Non-quarter-wave dielectric mirror prepared by thermal atomic layer deposition

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In this work we design and fabricate from $n(\lambda)$ and $k(\lambda)$ experimental data for both Al₂O₃ and TiO₂ single layer materials, an optical coating as “dielectric-mirror” following the stack formula (HxLy)8Hx. Optical coating based on multilayer film on BK7 glass and Si(100) wafer substrates, was growth by atomic layer deposition (ALD) at 150 °C. The optical constants and optical properties of Al₂O₃ - TiO₂ multilayer stack before and after thermal treatment at 450 °C were studied via spectroscopy ellipsometry and Uv – vis measures in the spectral range between 200 to 1100 nm, also similar samples were studied through TEM, SEM and AFM at room temperature in order to obtain information about the morphological properties. From optical studies, we found a rejected zone or “stopband region” between 369 - 464 nm as well as cut - off points at 364 and 488 nm respectively and the presence of an acceptable bandwidth for rejected zone at $\lambda_0 = 420$ nm reference wavelength. Results opens possibility to coat complex substrates, without direct evaporate expose-view, due to the conformably advantage from ALD technology and their affinity with integrated nanotechnology (microdevices) applications.

Keywords: Optical coating; multilayers stacks; dielectric mirror atomic layer deposition.

Acknowledgment: This work was partially supported by Dirección General de Asuntos del Personal Académico DGAPAUNAM, through research projects: PAPIIT IN112117, IN110018, IA101018, PAPIIME PE101317, PE100318 and FORDECYT - CONACYT 272894 project.

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Abstract ID: 503

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biodetection

Keywords: Fouling-resistant electrodes, heterogeneous electron transfer, aging

Thermally Modified Graphites for Fouling-Resistant Electrodes

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Adsorbents interfere with the surface chemistry of carbonaceous materials employed in electrochemistry by oxidation-induced aging diminishing the heterogeneous electron transfer (HET) kinetics. Now a thermal treatment protocol was employed on pyrolytic graphites and graphite felt. The treatment inhibited the growth of surface oxides and hydrocarbons on these graphite materials for at least 72 hours as gleaned from FTIR measurements. Further air exposure showed that even though surface functionalities would eventually form on the surfaces of these materials, the electrochemistry of these materials indicated that they experienced only limited air oxidation, with minimal decrease in their HET kinetics after 9 weeks to 10 months. The study of their electronic properties at the HOMO level suggested that band gap opening, as expected from a displacement of the Fermi edge from the Dirac points, was not responsible for the resistance of the electrodes to air-aging. Rather, a ratio of the π to σ peak intensities indicating a strongly correlated electronic nature, explained by the Hubbard model, is suggested to be responsible for the resistance to aging. The study suggests that freshly treated graphites could be deployed as adsorbent-free surfaces and overall, the graphite electrodes from this treatment protocol could be applied as fouling-resistant electrodes for example, as sensors in harsh, electrode-fouling environments.

Abstract ID: 504**Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)****Keynote**

Topics: Synthesis, Controllable Growth and Characterizations

Keywords: Key Words : Graphene, Preparation, Devices, Electronic properties

Controlled preparation of graphene and its electronic properties**Yunqi LIU**

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Graphene is a kind of two-dimensional π -conjugate material, which is a sheet of carbon atoms bound together with double electron bonds (called a sp^2 bond) in a thin film only one atom thick. At present, controllable and massive preparation of high quality graphene, property modulation (e.g. open up the energy gap), etc. still remain the bottleneck problems in terms of its practical applications. In this regard, we carried out comprehensive and deepening research, and a few representative results are as follows.

We proposed a new concept for the growth of graphene by using liquid Cu as a catalyst in chemical vapor deposition (CVD) method.¹ Uniform single-layered, self-aligned, large-sized, single-crystal HGFs and continuous monolayer films were prepared. We synthesized the N-doped graphene by a CVD method using NH_3 as N source, that was the first experimental example of the substitutionally doped graphene. Electrical measurements show that the N-doped graphene exhibits an n-type behavior, indicating substitutional doping can effectively modulate the electrical properties of graphene.^{2,3} We developed an oxygen-aided CVD process for synthesizing high-quality polycrystalline graphene on a large scale. Graphene can be directly synthesized on dielectric substrates, which can be directly incorporated into field-effect transistor fabrication.⁴⁻⁶ By using single-crystal graphene growth on a Cu surface as a model system, we demonstrate that trace amount of H_2O and O_2 impurity gases in reaction chamber is a key for the large fluctuation of graphene growth.⁷

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Thursday, 22/Aug/2019 5:03pm - 5:18pm

Abstract ID: 505 / FESC-2: 16

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Plenary

Topics: Artificial photosynthesis

Keywords: CO2 reduction, Graphene, Nano, photoconversion

Photoconversion of CO₂: Controllable Transition from C₁ to C₂ Products

SU-IL IN

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Photocatalytic reduction of CO₂ to fuel offers an exciting opportunity for helping to solve current energy and global warming problems. Although a number of solar active catalysts have been reported, most of them suffer from low product yield, instability, and low quantum efficiency. Therefore, the design and fabrication of highly active photocatalysts remains an unmet challenge. We seek CO₂ photoconversion efficiencies large enough for translation of the technology from laboratory to industry, a key step of which is achieving higher-order hydrocarbon products. Ethane, C₂H₆, for example, can be relatively easily converted into ethanol, a liquid fuel. In the current work, under AM1.5G illumination, utilizing a photocatalyst of reduced titania, graphene, and Pt nanoparticles, we demonstrate stable operation, significant rates of product formation, as well as a controllable product transformation from CH₄ to C₂H₆. We find the switch from C₁ to C₂ products is dependent upon upward band bending at the reduced blue-titania/graphene interface.

Abstract ID: 506

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Photocatalysis

Keywords: Carbon Nitride, Photocatalysis, Metal-to-Ligand Charge Transfer, Broad-Spectrum-Active

Photocatalytic hydrogen evolution under a broad solar spectrum based on effect between metal and ligand

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It is of great significance to fabricate a full-spectrum-active photocatalyst for the development of solar energy.¹ Graphitic carbon nitride (g-C₃N₄) is a kind of promising photocatalyst due to its photocatalytic stability and activity but its ability of absorbing light at $\lambda > 500$ nm is restricted. The Metal-to-ligand charge transfer (MLCT) mechanism was utilized by Xiong and his co-workers to broaden the light absorption range of g-C₃N₄.² This rational strategy created a narrow-energy-gap pathway for photo-generated electrons transfer but remains challenging to overcome the potential shortages, including recombination of photo-generated electron-hole pairs and small specific surface area. We developed a novel photocatalyst based on g-C₃N₄ via an improved MLCT mechanism. 1,2,4,5-Benzenetetracarboxylic acid (BTEC) with strongly-delocalized π electrons was coordinated onto g-C₃N₄ nanosheets via the copper (II) center. This constructed structure was both experimentally and theoretically proved to create three narrow-energy-gap electron transfer pathways (1.22 eV, 2.01eV and 2.39 eV respectively) in the material, which facilitated the absorption of light at $\lambda < 1100$ nm. The material exhibited outstanding photocatalytic activity under visible light and simulated solar light. Notably, the photocatalytic activity and apparent quantum efficiency was also acceptable under near-infrared light (at $\lambda > 800$ nm). The mechanism of both photocatalytic activity and stability was proposed based on this improved MLCT mechanism. This study offers a promising route to greatly enhance the optical properties of semiconductors and provides suggestive insights for engineering broad-spectrum-active and ultra-stable photocatalysts.

Wednesday, 21/Aug/2019 6:00pm - 6:12pm

Abstract ID: 507 / FBB: 11

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: 3D Scaffolds

Keywords: self-assembling peptide, 3D-printed scaffolds, biomimetic scaffolds, osteochondral regeneration

Nano-patterned Bilineage Scaffolds Coated by Self-assembly Peptide Hydrogels for Simultaneous Osteochondral Regeneration

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Clinically, cartilage damage is frequently accompanied with subchondral bone injuries caused by disease or trauma. However, the construction of biomimetic scaffolds to support both cartilage and subchondral bone regeneration remains great challenges. Herein, a novel strategy is adopted to realize the simultaneous repair of osteochondral defects by employing a self-assembling peptide hydrogel (SAPH) FEFEFKFK (F, phenylalanine; E, glutamic acid; K, lysine) to coat onto 3D-printed polycaprolactone (PCL) scaffolds. Results show that the SAPH-coated PCL scaffolds exhibit highly improved hydrophilicity and biomimetic extracellular matrix (ECM) structures compared to PCL scaffolds. In-vitro experiments demonstrate that the SAPH-coated PCL scaffolds promote the proliferation and osteogenic differentiation of rabbit bone mesenchymal stem cells (rBMSCs) and maintain the chondrocyte phenotypes. Furthermore, 3% SAPH-coated PCL scaffolds significantly induce simultaneous regeneration of cartilage and subchondral bone after 8 and 12 weeks, respectively, of in-vivo implantation. Mechanistically, by virtue of the enhanced deposition of ECM in SAPH-coated PCL scaffolds, SAPH with increased stiffness facilitates and remodels the microenvironment around osteochondral defects, which may favor simultaneous dual tissue regeneration. These findings indicate that the 3% SAPH provides efficient and reliable modification on PCL scaffolds and that SAPH-coated PCL scaffolds appear to be a promising biomaterial for osteochondral defect repair.

Wednesday, 21/Aug/2019 6:36pm - 6:48pm

Abstract ID: 508 / FCM: 14

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Thermal problems on Composite structures

Keywords: thermal management, graphene, epoxy, boron nitride, electrical conductivity

Enhancing Thermal Conductivity of Polymers

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The rapidly increasing device densities in electronics dictate the need for efficient thermal management. If successfully exploited, graphene, which possesses extraordinary thermal properties, can be commercially utilized in polymer composites with ultrahigh thermal conductivity (TC). The total potential of graphene to enhance TC, however, is restricted by the large interfacial thermal resistance between the polymer mediated graphene boundaries. We report a facile and scalable dispersion of commercially available graphene nanoplatelets (GnPs) in a polymer matrix, which formed composite with an ultrahigh TC of 12.4 W/m K (vs 0.2 W/m K for neat polymer). This ultrahigh TC was achieved by applying high compression forces during the dispersion that resulted in the closure of gaps between adjacent GnPs with large lateral dimensions and low defect densities. We also found strong evidence for the existence of a thermal percolation threshold. The addition of electrically insulating boron-nitride nanoparticles to the thermally conductive GnP-polymer composite significantly reduces its electrical conductivity (to avoid short circuit) and synergistically increases the TC. Indeed, when applied as potting (encapsulating) material for electronic devices, these novel hybrid composites effectively dissipate the heat; their operating temperatures decrease from 110 C to 37 C and their effective thermal resistances are drastically reduced, by up to 90%. The efficient dispersion of commercially available GnPs in polymer matrix provides the ideal framework for substantial progress toward the large-scale production and commercialization of GnP-based thermally conductive composites.

Abstract ID: 509 / Poster: 33

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Composite structures in civil engineering

Keywords: Particle-reinforcement, Plates, Mechanical properties, Rheological properties, Cement nanocomposites.

Reinforcement and workability aspects of graphene-oxide-reinforced cement nanocomposites

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Nanocarbons such as nanotubes or graphene have been employed to enhance the performance of cementitious composites due to their extraordinary mechanical and transport properties. Specifically, the use of hydrophilic graphene oxide (GO) is of great potential due to its compatibility with the water-based cement matrix. However, the addition of GO (or other nanocarbon fillers) to the cement matrix results also in increased viscosity, which reduces its workability and jeopardizes its casting process. We explored the mechanical and the rheological properties of cement reinforced with GO, in the presence of a superplasticizer. The GO enhanced the compressive and flexural strengths of the cement matrix by 40% and 70%, respectively, at extremely low GO concentrations (< 0.05 wt%). An optimal nanomaterial concentration (ONC) was observed, above which the properties deteriorate due to the formation of voids in the composite. In a comparison of different nanofiller-reinforced systems, the superiority of the cement + GO + superplasticizer system over other previously reported systems was shown by comparing the nanofiller reinforcement efficiency and a figure of merit that combines the nanocomposite's mechanical and rheological properties.

Abstract ID: 510

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Concrete and cementitious composites

Keywords: self-healing behavior, strain hardening cementitious composites, cementitious capillary crystalline waterproofing materials

Effect of cementitious capillary crystalline waterproofing materials on self-healing behavior of strain hardening cementitious composites

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Studies have shown that strain hardening cementitious composites (SHCCs) have the fine saturated and multi-crack characteristics, which make SHCCs have well self-healing potential. Concrete cracks are repaired well by cementitious capillary crystalline waterproofing materials (CCCW). The self-healing behavior of SHCCs incorporating CCCW was investigated. Three mixes, including control mix (FJ-0), 1.5% (FJ-1.5), 3% (FJ-3), were used. Uniaxial tensile test and capillary water absorption test were conducted to assess the recovery of mechanical and transmission properties. The experimental results show all specimens exhibit the strain-hardening characteristics after self-healing. Tensile property of specimens with CCCW was recovered well. With the amount of CCCW increasing, crack width of SHCCs was reduced and self-healing property was improved. Especially, FJ-3's tensile property exceeded the original value and the water absorption coefficient decreased by 56.12% after self-healing. The mechanism of the effect of CCCW on self-healing property of SHCC can be attributed to the fact that active material in the CCCW react with Ca²⁺ to form a water-insoluble white crystal precipitation filling the cracks. This study offers a promising route to greatly enhance the self-healing property of SHCCs, which is beneficial for improving the long-term performance of structures.

Thursday, 22/Aug/2019 12:15pm - 12:30pm

Abstract ID: 511 / FLNM-2: 7

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

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

Keywords: 2D materials, degradation. Tunable photoluminescence, black phosphorus oxide, 2D laser treatment.

Van der Waals Semiconductors: Towards New and Emerging Electronic and Photonic Devices

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Low dimensional materials have captured the attention of scientist and engineers. Owing to their layer dependent band gap, high electron mobility, and exceptional thermoelectric properties, 2-Dimensional materials have been the focal point of several research for various electronic and photonic applications. In my talk, I will show our recent results on laser treated MoS₂ nanosheets using Raman spectroscopy [1]. These MoS₂ nanosheets exhibit anomalous particle formation on the surface after laser irradiation. Our results demonstrate monolayer MoS₂ exhibit different behavior than few layers MoS₂, which is attributed to the observed different Raman characteristics after laser irradiation. Moreover, I will show our recent results on black phosphorus degradation using fast-scanning Raman spectroscopy [2]. We show a universal intensity modulation in all black phosphorus Raman modes with increasing degradation time. This observed intensity modulation is attributed to Raman scattering interference with incident laser beam, which can be used to extract the etching rate of black phosphorus nanosheets. Also, we demonstrate broadband tunable light emission (photoluminescence) out of layered black phosphorus using a new thermal technique. This light emission can be tuned between 590nm-720nm with 5nm spectral resolution. We attribute this observed light emission to the formation of stable black phosphorus oxide. The bandgap of this black phosphorus oxide can be tuned using this thermal technique. Finally, I will show our recent results on HfSe₂ material. This material is known to be n-type. However, our results show HfSe₂ FET devices exhibit an anomalous p-type behavior after laser treatment and electrical annealing. The origin of this anomalous p-type behavior is still not clear. Nevertheless, possible reasons include contact doping and the formation of thin oxide layer on the surface of HfSe₂. I will finally conclude with future outlook of layered 2D materials in photonic and electronic applications.

Thursday, 22/Aug/2019 2:15pm - 2:27pm

Abstract ID: 512 / FCM-4: 2

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Porous and cellular materials

Keywords: Lignin, Network Composite, Controllable Superabsorbent

Lignin-based and disulfate-linked aerogel as a selective, controllable, reusable superabsorbent

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Oil spills and organic contaminant have arisen serious problems on aquatic ecosystem. Network polymers or composites due to their tunable functionalities and controllable pore geometry has been attracted a lot of interest as the superabsorbent to remove oil and organic solvent from water. However, the complicated and harsh synthesis routes and expensive catalyst for network polymer prevents its further development. Herein, a selective and reusable oil superabsorbent was successfully prepared by a mild synthesis method using sustainable lignosulfonate (ELS) as a starting material, which can be reclaimed from waste stream of biorefinery or papermaking process. The modified ELS, trimethylolpropane tris(3-mercaptopropionate) (TMMA) in dimethyl sulfoxide (DMSO) catalyzed by sodium hydroxide (NaOH) in the presence of small amount of water via high density reverse-emulsion polymerization method followed by a freeze dry. The formation of disulfide-linked network composite was confirmed by Fourier transform infrared (FTIR) and ¹³C-NMR spectroscopy. The water-repellent and thermal stable absorbent sponge with a controllable pore geometry were further characterized by thermal gravimetric analysis (TGA), scanning electron microscopy (SEM), and Brunauer–Emmett–Teller (BET). The oil/organosolv removal capacity was performed in different contact times and oil/water mixture, and the sponge showed hydrophobic property as well as high adsorption capacity up to 2.6g oil/g absorbent for vegetable oil. And it also showed selective removal capacity for organic solvents. This work paves the way for a low cost, reusable, stable absorbent from lignin with excellent performance even in high oil concentration.

Abstract ID: 513

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Optical, electrical and magnetic properties of thin films

Keywords: thick-film resistors, substrate, glass ceramic, compatibility

Study on compatibility between thick-film resistors and fluorophlogopite glass-ceramic substrate

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Thick film resistors (TFRs) have great potential to be applied as strain sensors in civil engineering for the advantages of good sensitivity, stability, low cost, mass production, and long life. However, the usual alumina ceramic substrate with large elastic modulus (300~400GPa) is not suitable for strain monitoring, especially for civil engineering structures. In previous studies, we have shown that TFRs on fluorophlogopite glass-ceramic (FGC) are suitable for applying in strain monitoring of concrete because of comparatively low elasticity modulus(50~70GPa). For more extensive application of FGC substrate materials, the compatibility between the resistor paste and FGC substrate should be studied in detail. To this end, the TFRs fired FGC substrates were investigated with the aim of determining the compatibility of the resistor materials which were developed for firing on Al₂O₃, with FGC substrates. Resistor pastes (RuO₂ concentration range from 10 wt% to 30 wt%) were screen printed and sintered on FGC, and alumina ceramic (as a control) substrates. Sheet resistivities, temperature coefficients of resistance (TCRs) and gauge factors (GFs) of TFRs fired on FGC and alumina ceramic substrate were studied. The microscopic analysis results indicate that the properties of TFRs on FGC were determined by the diffusion and co-melting between glass in the resistor layer and substrate. For most resistors (RuO₂ concentration range from 10 wt% to 25 wt%), the diffusion of glass phase from the resistor layer into the FGC during firing which could increase the concentration of the conductive phase in the resistor leading to lower sheet resistivities, more positive TCRs and lower GFs. When the concentration of RuO₂ increases to 30%, TFRs on FGC have higher sheet resistance and GF, compare to the Al₂O₃ substrate. The reason is that the glass-ceramic substrate is co-melted with the glass, resulting in an increase in the glass content in the resistive layer.

Abstract ID: 514 / Poster: 27

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Processing and manufacturing technologies

Keywords: Reverse micelle, Stretchable, Adjustable, Elastomer, Filler-Matrix composites

An elastomer for epidermal electronics with adjustable adhesion force and stretchability obtained via a reverse-micelle-induced process

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Our work will give new insights and possibilities to filler-matrix composites. The key claim is to form and arrange the spots where the fillers are locally concentrated in the composite through the reverse-micelle induced process. The reverse-micelle envelop and deliver the filler into the matrix, and its degree of dispersion and volume of spot are controlled by the amount of emulsifier and filler.^{1,2} This is a new way of fine-tuning the filler that can be used as a tool to change the properties of the material as well as study the effects of the filler. To demonstrate the reverse-micelle induced process, we made an elastomer for epidermal devices. Through the process, the elastomer can readily control and extend range of the properties, adhesion force (0.014–1.1 N cm⁻¹), Young's modulus (16–535 kPa), and stretchability (430–1340%) while durability was maintained (stable upto 10,000 stretching cycles at 100% strain).² Furthermore, the elastomer is reusable and adheres well to human skin. Even when the skin is wet, the adhesion force is maintained at 80%. The all-solution-based process is compatible with low-cost, large-scale manufacturing.

Abstract ID: 515

Symposium 3: Functional Catalysis (FC)

Keynote

Topics: Photocatalysis

Keywords: Metal-Organic Framework, Photocatalysis, Photoelectronic Property, Confined Effect

Supramolecular Photocatalysis within Confined Environment of Metal-Organic Framework

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Photocatalysis is one of the most important chemical methods to mitigate the energy and environmental crisis via converting inexhaustible solar energy into clean chemical potential. The general history of the development of photocatalysis based on porous metal–organic frameworks (MOFs) is simply divided into three branches with a focus placed on the distinct structural role of the photocatalytic center: the inorganic cluster nodes, the organic linkers, and the guests in the pores of MOFs. In each branch, these photocatalytic centers are considered to be monodispersed within the crystal lattices with the other two structure roles regularly distributed to isolate the active centers and sometimes to provide more functions other than photoactivity. This distinctive nature has rendered MOFs as promising candidates for photocatalysis not only because they combine the benefits of heterogeneous catalysis and homogeneous catalysis but also because they facilitate the possibility of merging multifunctional catalytic sites for concerted or cascade photocatalysis. The design strategy and improvement approaches for MOF-based photocatalysts are also introduced with an emphasis on structure. Our intention is for this comprehensive view of MOFs-involved photocatalysts to inspire new ideas for designing heterogeneous photocatalysts toward the better utilization of solar energy.

Abstract ID: 516

Symposium 3: Functional Catalysis (FC)

Invited Talk

Topics: Photocatalysis

Keywords: Metal-Organic Framework, Photocatalysis, Radical Reaction, Confined Effect

Tackling Unusual Selectivity of Photocatalytic Trifluoromethylation for Protection of Metabolic Sites of Drugs by Enzyme-Mimicking Dye-based Metal-Organic Frameworks

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Photocatalytic trifluoromethylation of drug candidates selectively at metabolically susceptible positions is highly desirable in pharmaceutical applications, but the discrimination of various aromatic positions without distinct electronic contributions is thermodynamically difficult due to the high electrophilicity of CF₃ radicals. By combining triphenylamine (TPA)-derived ligands with invariable valence metal zinc or variable valence metals like copper, a new approach was designed to construct a series of metal-organic frameworks that are heterogeneous photocatalysts for the trifluoromethylation-initiated tandem reactions of unsaturated olefins. The derivatization of TPA well-tuned the photoreductive potential and ground state oxidative potential of MOFs, and the incorporation of chiral auxiliary to the ortho-positions of coordinative carboxylic moieties switched the electron transfer route of excited state, and also forged enzyme-like local environments within MOF cavities. The coordinative vacancies of metal nodes and other noncovalent interaction sites docked the substrates, and the copper clusters assisted to bind the radical species, the comprehensive effect of those factors benefited to tackle the photocatalytic trifluoromethylation and related tandem reactions with unusual chemo-, regio-, and stereoselectivities, and this methodology was also primarily utilized in the specific protection of metabolic sites of some drug candidates.

Abstract ID: 517

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Materials of Optical Coating

Keywords: Metal-Organic Framework, encapsulation, Epitaxial Growth

Epitaxial Growth and Application of Oriented Metal-Organic Framework Thin Film

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As multilayer materials with nanometers in thickness, metal-organic framework (MOF) thin films have been increasingly investigated due to their potential applications in molecular recognition/separation, catalysis, sensors and devices. In this work, we will summarize recent works focusing on epitaxial growth and applications of surface-mounted MOF thin films (SURMOFs) and encapsulated SURMOFs on substrate surfaces. Such oriented, compact and homogenous thin films provide a promising model for studying the crucial intrinsic properties in coordination chemistry, growth mechanism, chiral chemistry and the guest diffusion behavior in MOFs system. Their related applications on molecular adsorption and separation, optical applications, organic field effect transistors and catalysis are also described in this review. This review will be of interest to researchers on attempting to design other multifunctional MOF thin films and those engage in the extension of thin films to particle applications of sensors and devices.

Thursday, 22/Aug/2019 11:51am - 12:03pm

Abstract ID: 518 / FLNM-2: 5

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Spectroscopy studies of low dimensional, nano and 2D materials Carbon Based materials

Keywords: Graphene, Size effects, Spintronics

Size effects and electronic properties of graphene-based systems

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Wide class of nano-carbons are of a current interest due to their unconventional properties and potential applications in nanotechnology and nanoelectronics (spintronics). Quasi-graphitic systems such as GO, rGO or activated carbons (AC) built of the graphene nanoparticles exhibit specific electronic transport properties in which the size effects play a crucial role. Spin and charge localization in such systems strongly depends on the structure (texture) where individual graphene-like particles are separated by potential barriers. These barriers define the size of such particles and are responsible for the localization effects within them. Specific guest molecules located in such systems can enhance these effects and help to control the conducting properties locally as well as on macro-scale.

We report the observation of electronic properties of a few graphene-based systems (GO, rGO, AC) modified by chosen guest molecules, performed with the electron paramagnetic resonance, resistivity measurements and Raman spectroscopy. The results are discussed in a frame of the granular metal model, proposed for the activated carbon fibers [1] and other carbon nanocrystalline materials [2-4], where the strong localization of spin and charge leads to the hopping transport.

Key Words: Graphene, Size effects, Spintronics

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Abstract ID: 519

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Magnetic Materials

Keywords: magnetism, 2D materials, exfoliation, spin glass

Uncovering anisotropic magnetic phases via fast dimensionality analysis

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Here we present how our quantitative geometric predictor for the dimensionality of magnetic interactions can guide the synthesis of new compounds and the selection of functional layered magnets. This predictor is based on networks of superexchange interactions and can be quickly calculated for crystalline compounds of arbitrary chemistry, occupancy, or symmetry. The resulting data are useful for classifying structural families of magnetic compounds. We have examined compounds from a demonstration set of 42 520 materials with 3d transition metal cations. The predictor reveals trends in magnetic interactions that are often not apparent from the space group of the compounds, such as triclinic or monoclinic compounds that are strongly 2D. We present specific cases where the predictor identifies compounds that should exhibit competition between 1D and 2D interactions, and how the predictor can be used to identify sparsely populated regions of chemical space with as-yet-unexplored topologies of specific 3d magnetic cations.

Abstract ID: 520

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Ceramic based composites

Keywords: Porous alumina ceramic; Graphite waste; Porosity; Mechanical properties; Ceramic matrix composite.

Fabrication and Properties of Porous Alumina Ceramics Using Graphite Waste as a Pore Forming Agent

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Porous alumina ceramic materials have been fabricated using a new industrial waste i.e. graphite waste from primary batteries. This is used as a pore-forming agent by means of a fugitive materials technique. The pore agent ratios ranged from 10 to 50 wt %. The results showed that by increasing the graphite waste content from 10 to 50 wt %, the porosity increased from 37.27 to 61.08 % and the mechanical properties decreased. The hardness decreased from 172.64 to 38.12 HV1 while the tensile strength and the compressive strength decreased from 24.97 to 14.28 MPa, 112.25 to 34.28 MPa respectively. The graphite waste material was successfully used as a pore-forming agent to produce porous alumina ceramic materials. The decrease in the mechanical properties was connected to the increase in porosity with the addition of the pore agent ratio. This research study has promoted several practical applications such as hot gas filters and molten metal filters.

Keywords: Porous alumina ceramic; Graphite waste; Porosity; Mechanical properties; Ceramic matrix composite.

Abstract ID: 521

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Fuel Cells

Keywords: Solid oxide fuel cell, interconnect, FeCr ferritic steel, plasma nitriding, electrical resistance

Using pulsed plasma nitriding to improve the conductivity property of SOFC interconnect made from ferritic FeCr steels

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Solid oxide fuel cell (SOFC) has stepped into various industrial applications owing to its excellent energy conversion efficiency. However, the SOFC interconnect made from Fe-Cr based ferritic stainless steel suffers from preferential oxidation to form chromia oxide which triggers poor electrical conductivity and Cr-poisoning to the SOFC cathodes. To overcome this drawback, research has been made by novel FeCr alloy design expecting the formation of a spinel-type oxide scale or by the deposition of a spinel-type topcoat. In this presentation, we report an alternative technique to prevent the chromia oxide. Several FeCr stainless steels were treated by pulsed direct-current glow discharge plasma nitriding in an Ar-N₂ atmosphere. The nitriding treatment led to an approximately 60 μm thick nitrided layer containing up to 10 wt% of nitrogen and having a multiphase structure of CrN, Cr₂N and Fe₄N. The electrical interface conduct resistance (ICR) of both the nitrided and non-nitrided FeCr foils were measured after annealing the samples in air for 8 hours at various temperatures up to 900°C. The nitriding treatment has been found to reduce the ICR values by 60% over a wide range of elevated temperatures up to 700°C. This performance is expected to ensure good electrical conductivity of SOFC devices. The mechanism of the improved ICR property was comprehensively investigated by field-emission scanning electron microscopy, energy dispersive X-ray spectroscopy, Raman spectroscopy and X-ray diffraction. As expected, annealing of bare FeCr steel foils resulted in a dense top layer of chromia. In contrast, hematite Fe₂O₃ became the leading oxide phase on the annealed nitrided FeCr steel foils. This dramatic change in the surface oxide brought about the lower ICR, which was attributed to the role of nitrogen in chemically blocking chromium atoms in the resultant CrN and Cr₂N compounds.

Abstract ID: 522

Symposium 2: Functional Composite Materials (FCM)

Keynote

Topics: Dielectric, Ferroelectric and Piezoelectric materials

Keywords: Multiferroics, Antiferroelectrics, Ferromagnetism, Magnetodielectric coupling effect

Antiferroelectric and Magnetodielectric Coupling Response of La_{0.2}Sr_{0.7}Fe₁₂O₁₉ Ceramics

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Multiferroics is a class of functional materials that simultaneously exhibit ferroelectricity and ferromagnetism in a single structure. We report here the integration of anti-ferroelectricity and ferromagnetism in a new M-type hexaferrite compound with a formula of La_{0.2}Sr_{0.7}Fe₁₂O₁₉, in which 0.3 Sr ions were substituted by 0.2 La³⁺ ions in SrFe₁₂O₁₉ so as to keep the charge balance. XRD results show a lattice contraction of 0.59% in comparison with SrFe₁₂O₁₉. Surprisingly, the doping effect turns La_{0.2}Sr_{0.7}Fe₁₂O₁₉ from ferroelectric to antiferroelectric phase, which displays double hysteresis loops with a saturated polarization of 154 $\mu\text{C}/\text{cm}^2$ and a remnant one of 38 $\mu\text{C}/\text{cm}^2$. This compound simultaneously demonstrates strong ferromagnetism, the remnant magnetic moment and coercive field are measured to be 52 emu/g and 5876 Oe, respectively. Meanwhile, La_{0.2}Sr_{0.7}Fe₁₂O₁₉ also exhibits strong magnetodielectric (MD) response, an applying magnetic field (B) lifts the whole ϵ' -f spectra up and right shifts ϵ'' -f spectra (ϵ''_m) to higher frequency side. Both frequency-dependent real and imaginary parts of the dielectric constant obey Debye relaxation model and vary with B field at a large amplitude. The maximum MD increment in ϵ' reaches as high as 540830 upon a B field of 926mT. The capacitance of the La_{0.2}Sr_{0.7}Fe₁₂O₁₉ ceramics has been much more enhanced by applying a magnetic field B, which induced an additional polarization P(H) upon the conventional P(E) by cycloid conical spin in the intermediate phases. These results suggest that La_{0.2}Sr_{0.7}Fe₁₂O₁₉ could exhibit a strong interplay between magnetic ordering and ferroelectricity, which makes it a good multiferroic candidate with strong magnetoelectric coupling effect.

Abstract ID: 523

Symposium 6: Functional Thin Films (FTF)

Invited Talk

Topics: Protective Coatings in Severe Environments

Keywords: Graphene, Nomposite, Electro-plating, Coating, Corrosion resistance

Preparation of Metal-Gr Composite Coatings via Electro-plating for High Corrosion Resistances

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1. Preparation of Fe-Gr composite coating via DC electro-plating for high performances

In this work, the iron-graphene (Fe-Gr) composite layer was prepared by using an electro-plating method. The performance of the composite was varied with the concentrations of GO in the electrolyte. The layer's microstructures were systematically characterized by SEM, TEM, Raman, FT-IR, and the micro-hardness and its corrosion resistance were evaluated for getting desired properties. The experimental results revealed that: 1) the Gr could be scattered homogeneously in the Fe layer when dispersible graphene oxide (GO) was added in the electrolyte; 2) comparing with pure Fe layer, the micro-hardness and corrosion resistance of the Fe-Gr composite layer were greatly enhanced; 3) it was found that there was an optimal GO additive amount (0.4 g/L) in the electrolyte, which increased the properties involving the micro-hardness up to HV 248, 2.07 times higher than that of pure iron layer(HV 120); 3.75 times of anti-corrosion rate(0.1353 mmy-1) and 5.38 times of the charge transfer resistance(1456 /($\Omega \cdot \text{cm}^2$) higher than that of pure iron layer(0.5076 mmy-1, 270.5 /($\Omega \cdot \text{cm}^2$)).

2. Preparation of Zn-Gr composite coating via pulse reverse electro-plating for high corrosion resistances

In this work, a kind of the Zn-Gr composite layer is successfully prepared on iron substrate via pulse reverse electro-plating method from a chloride aqueous solution. The experimental results revealed that: 1) By adding GO in the electrolyte, Gr sheets can be incorporated homogeneously in the Zn plating layer during electro-plating, and the reduction from GO into Gr occurs due to the Zn and GO co-deposition. 2) Due to increasing of the nucleation sites, Gr incorporation changes the growth mechanism of Zn crystal, i.e., makes the main preferred orientations from (112) and (101) crystal planes in the pure Zn layer into (103), (102) and (110) planes in the Zn-Gr composite layers. 3) As a corrosion protection barrier layer, Gr sheets play an important role on the corrosion resistance of the Zn-Gr composite plating layers in simulated seawater environment. The highest corrosion resistant properties occur in an optimal range 0.3 – 0.5g/L GO adding amount in the electrolyte, at which the corrosion current density just be a hundredth comparing with that of pure Zn layer. 4) The present method for preparing Zn-Gr composite, with advantages of simple, controllable, scalable, etc., is likely to be industrialized.

Abstract ID: 524

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Fundamental investigations on low-dimensional nanomaterials and their functional structures properties

Keywords: graphene oxide, degree of reduction, charges storage, charges transfer, scanning polarization force microscopy

Charges storage and transfer behaviors of single layer reduced graphene oxide sheets

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As an attractive alternative to graphene, the reduced form of graphene oxide (GO) can be used for producing large-scale flexible devices that require an electronic gap. By controlling the reduction degree of GO, their electronic properties were tuned. Herein, scanning polarization force microscopy (SPFM) is used to distinguish the one-atom-thick GO and reduced GO (rGO) sheets and monitor the thermal reduction process in-situ. The reduction degree related electrostatic properties such as the charge storage character of nanostructured and partially reduced GO sheets are further studied by using the scanning probe microscopy (SPM) based charging and discharging technique and the sample-charged mode SPFM (SC-SPFM). Furthermore, charged nanostructures with controllable geometry and charge density are achieved with the thermal nanolithography method. Such charged nanostructures could be used to construct charge gated graphene nanoelectronics. In the last part, we will briefly report the effects of injected charges to adjacent rGO sheets, such as the inhomogeneous charges distribution in rGO sheet induced by adjacent charged ones and the charges transfer behavior between physically separated rGO sheets on insulating substrates. These effects are of great value for rational design of graphene nanoelectronics with desired functionality.

Tuesday, 20/Aug/2019 2:00pm - 2:45pm

Abstract ID: 525 / Keynote-2: 1

Symposium 2: Functional Composite Materials (FCM)

Plenary

Topics: Additive manufacturing Applications

Keywords: 4D printing, Multi-material, Smart structures, Shape change, Function variation.

Smart structures and 4D printing

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With progressive advancements in various cutting-edge technologies, smart structures with both robust stability and manipulatable functions are highly pursued to meet the critical requirements in the various complicated environments. On the other hand, development of additive manufacturing technology has fundamentally exhibited great advantages, which provides an exclusive platform for manufacturing smart structures. Based on 3D printing added with additional dimension, either time or space, for manipulating shape, property or functions, in the present talk, I would initially analyze the key scientific issues in 4D printing technology, including design, materials, apparatus, software, manipulation and applications. Based on an advanced multi-material structure strategy for achieving smartness, I would give several examples based on our current studies for better understanding how 4D printing plays a significant role in designing and manufacturing smart structures and smart devices. The 4D printing technology is expected to open up a novel strategy for substantially endowing the advanced structures with smartness and exceptionality.

Abstract ID: 526

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Mono-dispersibility, $\text{MnO}_2 \cdot 0.5\text{H}_2\text{O}$, Adsorb Capacity, Efficiency

Preparation of Uniformly Dispersed Mn-based Oxide Ion Sieves with High Adsorption Capacity and Selectivity for Lithium separation from Brine

Chunxi Hai^{1,2}, Guicai Qi^{1,2,3}, Yuan Zhou^{1,2}, Yue Shen^{1,2}, Yanxia Sun^{1,2}, Shengde Dong^{1,2,3}, Xiang Li^{1,2}

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Lithium ion-sieves is commonly regarded as the ideal candidate for the most promising material to extract of lithium from aqueous solution for industrial application. In this study, taking the high capacity, good chemical stability and low cost into consideration, meso-porous sphere-like $\text{MnO}_2 \cdot 0.5\text{H}_2\text{O}$ lithium ion-sieves with good dispersibility was prepared by employing $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$ which was synthesized by a facile solid-phase synthesis method by using synthesized Mn_2O_3 microspheres and commercial $\text{LiOH} \cdot \text{H}_2\text{O}$ as precursor. As-prepared sphere-like precursor spinel $\text{Li}_{1.6}\text{Mn}_{1.6}\text{O}_4$ not only has high adsorption capacity around 42.46 mg/g, but also plays an important role in controlling the lithium removal efficiency up to 90 %. Moreover, the Mn dissolve loss problem also can be effectively resolved by structure doping with Al.

Abstract ID: 527

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Anodes and cathodes Materials

Keywords: Ni-Co-Mn-Cd based precursor, solvothermal method, $\text{Li}(\text{Ni}_{0.6}\text{Co}_{0.2}\text{Mn}_{0.2}\text{O}_2)_x\text{Cd}_{1-x}\text{O}_2$, cathode materials

Solvothermal synthesis of $\text{Li}(\text{Ni}_{0.6}\text{Co}_{0.2}\text{Mn}_{0.2})_x\text{Cd}_{1-x}\text{O}_2$ cathode materials with excellent electrochemical performance

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The Ni-Co-Mn-Cd based precursor is initially synthesized by solvothermal method, and then the $\text{Li}(\text{Ni}_{0.6}\text{Co}_{0.2}\text{Mn}_{0.2}\text{O}_2)_x\text{Cd}_{1-x}\text{O}_2$ ($x=0, 0.01, 0.02$) cathode materials are prepared by high temperature solid phase method. The scanning electron microscope (SEM), X-ray powder diffraction (XRD), transmission electron microscope (TEM), and X-ray photoelectron spectroscopy (XPS) are used to determine the morphology, structure, elemental composition and electronic state of pristine and Cd-doped cathode materials. The electrochemical test indicates that Cd-doped samples exhibit better electrochemical performance than the pristine material, especially the doping amount of 0.01 mol, the discharge capacity can reach up to 186.3 mAh g⁻¹ with the capacity retention of 82.8% after 100 cycles at a current rate of 1 C, while the pristine material only has the capacity of 173.2 mAh g⁻¹ with the capacity retention of 69.8% at the similar current rate and cycle numbers. Meanwhile, even at 8 C, the discharge capacity is still up to 129.8 mAh·g⁻¹ at 8 C, however, the pristine material only has the capacity of 119.6 mAh·g⁻¹ at 8C. The enhanced electrochemical performance is attributed to the modification method by in-situ doping during the synthesis process of precursor effectively stabilizes the crystal structure and enhances the electronic conductivity of the material, as well as reduces the attack of HF on the electrode surface during the cycle process due to the generation of CdF.

Abstract ID: 528

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Anodes and cathodes Materials

Keywords: lithium-ion battery; Ni-rich layered $\text{LiNi}_{0.7}\text{Co}_{0.2}\text{Mn}_{0.1}\text{O}_2$; CeO_2 coating; cathode materials

Ultrathin CeO_2 coating for improved cycling and rate performance of Ni-rich layered $\text{LiNi}_{0.7}\text{Co}_{0.2}\text{Mn}_{0.1}\text{O}_2$ cathode materials

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In this study, we have successfully coated the CeO_2 nanoparticles (CeONPs) layer onto the surface of the Ni-rich layered $\text{LiNi}_{0.7}\text{Co}_{0.2}\text{Mn}_{0.1}\text{O}_2$ cathode materials by a wet chemical method, which can effectively improve the structural stability of electrode. The X-ray powder diffraction (XRD), transmission electron microscope (TEM), scanning electron microscope (SEM), and X-ray photoelectron spectroscopy (XPS) are used to determine the structure, morphology, elemental composition and electronic state of pristine and surface modified $\text{LiNi}_{0.7}\text{Co}_{0.2}\text{Mn}_{0.1}\text{O}_2$. The electrochemical testing indicates that the 0.3 mol% CeO_2 -coated $\text{LiNi}_{0.7}\text{Co}_{0.2}\text{Mn}_{0.1}\text{O}_2$ demonstrates excellent cycling capability and rate performance, the discharge specific capacity is 161.7 mAh g⁻¹ with the capacity retention of 86.42% after 100 cycles at a current rate of 0.5 C, compared to 135.7 mAh g⁻¹ and 70.64% for bare $\text{LiNi}_{0.7}\text{Co}_{0.2}\text{Mn}_{0.1}\text{O}_2$, respectively. Even at 5 C, the discharge specific capacity is still up to 137.1 mAh g⁻¹ with the capacity retention of 69.0%, while the NCM only delivers 95.5 mAh g⁻¹ with the capacity retention of 46.6%. The outstanding electrochemical performance is assigned to the excellent oxidation capacity of CeO_2 which can oxidize Ni^{2+} to Ni^{3+} and Mn^{3+} to Mn^{4+} with the result that suppress the occurrence of $\text{Li}^+/\text{Ni}^{2+}$ mixing and phase transition. Furthermore, CeO_2 coating layer can protect the structure to avoid the occurrence of side reaction. The CeO_2 -coated composite with enhanced structural stability, cycling capability and rate performance is a promising cathode material candidate for lithium-ion battery.

Abstract ID: 529

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Lithium Ion Batteries

Keywords: Lithium ion battery, cathode material, NCM811, doping modification, electrochemical performance.

**Effect of Na and Mg co-doping on Electrochemical Performance of Ni-rich
LiNi_{0.8}Co_{0.1}Mn_{0.1}O₂ Cathode Material for Lithium Ion Battery**

Yanxia Sun, Chunxi Hai, Yue Shen, Xiang Li, Shengde Dong, Yuan Zhou

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The Ni-rich layered material Li(Ni_xCo_yMn_{1-x-y})O₂ (x>0.6) is considered as the most promising cathode material for lithium ion batteries (LIBs) because of their high specific capacity. Unfortunately, the problem of Ni and Li cation mixed doping results in poor structural stability and poor rate and cycling performance for this type of materials. Degradation phenomena in NCM structures originate from various factors: lattice instability, cation disordering, phase transformation, microcrack propagation, and oxygen release from cathode side reactions. The doping method can improve these disadvantages. At present, the research on doping elements is single and insufficient.

It is considered that the appropriate doping of Na or Mg element has a positive effect on the electrochemical properties of the cathode material for lithium ion battery. So we have studied the influence of the Na and Mg mixed doping on the structure and electrochemical performance of Ni rich material LiNi_{0.8}Co_{0.1}Mn_{0.1}O₂. By the mixed doping of sodium and magnesium, the respective advantages of sodium and magnesium can be exerted, and synergistic effects are exerted, thereby improving the structural stability and rate performance of the material

Wednesday, 21/Aug/2019 5:00pm - 5:12pm

Abstract ID: 530 / FCM: 6

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: MOFs (metal-organic framework); self-assembly; MoS₂; composites; CO₂ adsorption

Self-assembly Composites of HKUST-1 MOFs with MoS₂ for CO₂ adsorption

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Novel ordered composites comprised of micropores and mesopores were synthesized by assembling HKUST-1 on MoS₂ nanosheet. The MoS₂/HKUST-1 was characterized using a combination of XRD, TEM, SEM, TPD, BET, CO₂ adsorption test, respectively. In this study, the amount of MoS₂ cores was demonstrated to influence the adsorption performance. The results suggest that the co-existence of MoS₂ could promote the formation of minimized-scale HKUST-1, and the addition of MoS₂ does not affect HKUST-1 structure. Furthermore, the micropore/mesopore volume ratio can be controlled by varying the amount of MoS₂ used. The CO₂ adsorption capacities were examined by CO₂ adsorption isotherm at 25°C. The CO₂ adsorption capacity of modified HKUST-1 reaches 21.21 wt%. All the original/modified HKUST-1 remain high CO₂ uptake in 10 times of adsorption/desorption cycles.

Wednesday, 21/Aug/2019 6:03pm - 6:15pm

Abstract ID: 531 / FC: 11

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalysis for pollution control

Keywords: g-C₃N₄; mercury removal; single-atom catalyst; Mn

Carbon nitride-support Single Mn atom as catalyst for Mercury removal in flue gas by first-principles calculations

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Elemental mercury(Hg⁰) emitted by coal-fired power plants is very harmful for human health, and it is urgent to develop cost-effective, high adsorption capacity and recyclable adsorbents to realize mercury control. Single atom catalysts(SACs) has receive considerable attention due to the excellent metal utilization. g-C₃N₄-based substrates exhibits unique properties as a support for single-atom heterogeneous catalysts.[1] The application of computational chemistry in understanding mercury removal mechanisms will help to modify and design mercury removal materials, thereby improving the efficiency of the removal of mercury in flue gas. In this work, we use first-principles calculations to systematically explore the potential of 3d-transition metals(Sc~Cu) embedded in the cavity of g-C₃N₄ as single-atom catalysts for mercury capture. The results show that all the metal atoms can be thermodynamically enter in the cavity while mercury could only be chemisorbed onto these metals by the order (Mn > Cr > Fe > Sc > Ti > Cu) the Sc, Ti, Cr, Mn, Fe and Cu sites. Thus, the mechanism of mercury adsorption on the Mn-doped surface is built, and the oxidation of Hg to Hg²⁺ under O₂ takes place through the E-R mechanism, where O₂ competes for Mn site with Hg⁰ and breaks down easily with the existence of mercury, later connecting the gas phase or a weakly adsorbed Hg⁰. This study offers a promising guide of single-atom catalysts to significantly improve the efficiency of the control of mercury pollution with g-C₃N₄-based support effects.

Abstract ID: 532

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalysis for pollution control

Keywords: environment, nanoparticles, hazardous, pollutants, photo-catalyst

Photo-catalytic Removal of Environmental Pollutants Under Solar Radiation Using High Band Gap Semiconductor Nanoparticles

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Our environment is being polluted with chemicals such as: dyes, phenols, pesticides and heavy metals due to the release of untreated industrial effluents and domestic sewage discharge. These chemicals, because of their toxic and non-biodegradable nature, are not only hazardous to human health but also degrade the eco-system. The techniques such as: adsorption, micro-filtration and use of coagulants for the treatment of contaminated water, are costlier, inefficient and generate a large amount of sludge as solid waste. However, photo-catalytic degradation of environmental pollutants using semiconductor nanomaterial, under solar radiation, can be a cost-effective and environment friendly alternative. Unfortunately, the commonly used high band gap photo-catalysts such as TiO₂ and ZnO for purifying contaminated water or air are photo-active only under ultra-violet radiation, thus are less efficient under the visible or solar light. Moreover, the high cost of the UV source, restricts the use of these photo-catalysts for the large scale treatment of wastewater. Therefore, in order to minimize the cost of photo-catalytic process, using high band gap semiconductors, diverse strategies have been adopted for enabling them visible light-sensitive and thus harvesting the inexpensive solar radiation. This paper highlights such strategies including: optimizing photo-catalyst nanosize and morphology, doping metals/non-metals, compositing two or more photo-catalysts and the use of sensitizers. Solar photo-catalytic reactors and parameters affecting the efficiency of photo-catalytic degradation of some pollutants have been described.

Abstract ID: 533

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Computational modeling and simulation of low dimensional, nano and 2D materials

Keywords: 2D perovskites, DFT, Strain, Electronic Structure, optical properties

MAPI monolayer with High Solar Efficiency: Ab-initio Method

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The 2D halide perovskite have distinct modulate compositional and structural tunable properties, which makes 2D materials as a good candidate to improve the characteristics of photovoltaic applications. We have explored strain dependent structural, electronic and optical properties of organic-inorganic hybrid perovskite Methylammonium Lead Halide (MAPI) monolayer using the density functional calculations. Here, we have calculated carrier mobility of electron and hole and the band gap of the MAPI monolayer. The results suggest that with increasing tensile and compressive strain, the band gap increases up to 5% (in tensile), while decreases towards instability i.e. 9% of compressive strain. The carrier mobility of MAPI monolayer is approximately 16 times larger than bulk MAPI. Furthermore, we have also investigated strain dependent optical properties, which show good activity in the visible as well as the high ultraviolet region of the spectrum. In addition, the MAPI monolayer shows high absorption coefficient at 8.8 eV is $14.09 \times 10^5 \text{ cm}^{-1}$ which is up to 40% higher than the bulk MAPI. For photovoltaic applications, we have calculated the open circuit voltage (Voc), fill factor (FF), short circuit current density (Jsc) and power conversion efficiency (η) of the MAPI monolayer. Our theoretical results suggest that the power conversion efficiency (η) is 28 % which is higher than its bulk form and 5% less than the Shockley-Queisser limit (33%), suggests that MAPI monolayer is a good candidate for the solar cell application.

Thursday, 22/Aug/2019 2:48pm - 3:00pm

Abstract ID: 534 / FTF-2: 5

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin Films in Photovoltaic Cells and Energy

Keywords: Silicon carbide film, PECVD, Photoelectrochemical water splitting

Amorphous silicon carbide thin films doped with P or B for the Photoelectrochemical water splitting devices

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Photoelectrochemical water splitting devices require semiconductor photoelectrode material fulfilling a number of primary requirements such as band gap, band edge alignment and corrosion resistance to electrolyte. Amorphous silicon carbide films (a-SiC:H) were deposited on Si substrates by plasma enhanced chemical vapor deposition (PECVD) technique using SiH₄ (100 %), CH₄ (100 %) and PH₃ (2 vol. % in H₂) or B₂H₆ (5 vol. % in H₂) as precursor gasses and H₂ as carrier gas. A RF generator with a frequency of 13.56 MHz was employed. Typical deposition parameters were 100 W, 100 Pa and 300 °C. The film thickness was typically about 250 nm. Three types of samples were prepared, one without doping and two with P or B doping. The concentration of elements in the films was determined by RBS and ERD analytical method simultaneously. Raman spectroscopy study of the SiC films were performed by using a Raman microscope with 532 nm laser and chemical compositions were analyzed by Fourier transform infrared spectroscopy (FTIR), before and after immersion of samples to aqueous pH 2.0 and pH 1.0 sulfuric acid electrolyte (200 h durability test). Electrical properties of SiC films before and after immersion of samples to aqueous pH 2.0 and pH 1.0 sulfuric acid electrolyte were studied by measurement of the I-V characteristics on structure Al/SiC/Si/Al. Amorphous silicon carbide films contain silicon, carbon, hydrogen, phosphorus or boron and small amount of oxygen. Differences between Raman spectra, FTIR spectra and I-V characteristics before and after immersion to electrolyte are discussed.

Abstract ID: 535

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Science of Thin Films and Quantum Effects

Keywords: Carbon thin film, Nano, Photo-electron emission

N-doped nanostructured carbon very thin films on quartz and sapphire substrate: Photo-electron emission properties

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Carbon-based materials have long been identified as a suitable thin film cathode for use in electron emitting structures. N-doped nanostructured carbon (ns-carbon) very thin films were deposited on quartz and sapphire substrate by RF (radio frequency) reactive magnetron sputtering using carbon target and gas mixture of Ar and reactive gas N₂. Carbon film was deposited at a working pressure 0.7 Pa and magnetron input RF power 150 W at 13.56 MHz. Argon and nitrogen flows were 30 sccm and 6 to 20 sccm, respectively. Substrate holder temperature during magnetron sputtering was in the range 500-900 °C. Deposited film thickness was in the range 10 to 30 nm. The concentration of elements in films was determined by RBS and ERD analytical method. Scanning Electron Microscopy (SEM) was used to investigate the surface morphology of ns-carbon thin films. Raman spectroscopy was used for determination of chemical-structural properties of ns-carbon thin films. Photo-induced electron emission method was used for the study of photo-electron emission properties of ns-carbon very thin films. Structure of ns-carbon thin films on quartz or sapphire as transmission photocathode was back-side illuminated with pulsed laser (266 nm) and measured bunch charge. N-doped ns-carbon films contain carbon, nitrogen and small amount of oxygen and hydrogen. SEM results showed no significant difference between sample surfaces. Raman spectra shapes are similar to GNDC (graphite-like nanocrystalline diamond) or BFG/UNCD (bristling few-layer graphite/ultrananocrystalline diamond composite film). Measured bunch charge results showed better photo-electron emission properties of ns-carbon very thin films prepared on sapphire substrates. Effects of substrate and technology of ns-carbon very thin films on the properties of photo-induced electron emitters as back-side illuminated transmission photocathode are discussed.

Abstract ID: 536

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Polymeric composites

Keywords: LDPE, perovskite ceramic, tensile properties, dielectric properties, ac impedance

Mechanical and AC Electrical Properties of Low-Density Polyethylene/BiSr₂CaCu₂O_{6.5} Thick Film Composites

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Low-density polyethylene (LDPE) has good chemical resistance and electrical properties, but it has some disadvantages such as poor heat resistance, very low stiffness, high coefficient of thermal expansion etc. In the present study, one of the Bi-based novel perovskite ceramic material was added to LDPE to improve its mechanical performance and electrical properties. The BiSr₂CaCu₂O_{6.5} (shortly Bi-1212) perovskite material was synthesized by the solid reaction method. The LDPE and Bi-1212 powders were mixed in the case where Bi-1212 is ranged from 0.5% to 6% by weight, and then the thick film LDPE / Bi-1212 composites were prepared by the hot press technique. The high-resolution images from the surface of the films were taken by scanning electron microscope. By using Fourier Transform Infrared (FTIR) Spectroscopy method, the chemical structures of the composites were also investigated. The mechanical properties of the samples such as Young's modulus, tensile strength, percentage strain at break and energy at the break were determined by Lloyd Instruments LF plus Single Column Universal Materials Testing Machine at room temperature. The improvement of the tensile parameters of LDPE due to Bi-1212 additive was also discussed. Additionally, it was observed that Young's modulus and stiffness of the LDPE are improved by the addition of 1% Bi-1212 additive. The alternative current (ac) electrical properties of the samples were measured by NOVO Control Broadband Dielectric/Impedance analyzer in the frequency interval of 10 Hz–40 MHz between 293 K and 353 K. The frequency and temperature dependence of the real and imaginary parts of the complex dielectric and impedance function of the LDPE were evaluated in terms of increasing Bi-1212 ceramic filler. It was determined that in accordance with the requirements of the technological application in which LDPE will be used, the dielectric constant of LDPE can be increased or decreased in a controlled manner.

Abstract ID: 537

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Catalysis for Chemical Synthesis

Keywords: N-doped mesoporous carbon, Nanomaterial, Heterogeneous catalyst, N-arylation reaction.

Pd nanoparticles immobilized on the poly-dopamine decorated halloysite nanotubes hybridized with N-doped mesoporous carbon sheet: A versatile catalyst for promoting N-arylation reaction

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Porous carbon materials have attracted considerable attention due to their applications in a wide range of areas, including energy storage and conversion, adsorption, catalysis, sensor technology, controlled drug release and cellular delivery. As an important class of novel porous carbons, N-doped mesoporous carbon materials have become a research hotspot due to their unique morphology, large surface area and pore volume, good electrical conductivity, and high physical and chemical stability. In recent years, with the rapid growth in the preparation and applications of N-doped mesoporous carbon [1], these materials present great utilitarian value for catalysis. Recently we designed and prepared several heterogeneous catalysts [2-4] and proving their utility for development for various chemical transformations under green conditions. In this line, we reported the outstanding effect of hybridization of Halloysite nanoclay with N-doped mesoporous carbon materials, graphitic carbon nitride (g-C₃N₄), on the catalytic activity and recyclability of the heterogeneous catalysts [2,3]. In continuation of our interest in the above mentioned achievements we focused on studying the effects of incorporation of N-doped carbon nanomaterials on the catalytic performance of the Halloysite nanoclay-based catalyst. In this regard, herein we wish to report our successful achievement on the preparation of an efficient heterogeneous catalyst so-denoted, Pd@Hal-pDA-NPC, which was prepared through immobilization of Pd nanoparticles on polydopamine decorated halloysite nanoclay (Hal-pDA) followed by incorporation of N-doped porous carbon monolayers (NPC). Then, we examined this novel composite fruitfully as an efficient heterogeneous catalyst in N-arylation of various organic compounds containing nitrogen. The catalyst exhibited excellent recyclability up to 10 consecutive reaction runs and low Pd leaching. Comparison of the catalytic activity of Pd@Hal-pDA-NPC with control samples confirmed the superior role of both p-DA and NPC in anchoring Pd nanoparticles, suppressing Pd leaching and consequently improving the catalytic performance of the catalyst.

Abstract ID: 538

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Keynote

Topics: Structural, Electronic, Optical and Magnetic Properties

Keywords: First-principles; Electronic structure; Optical properties; LaBr₃:Ce

Effect of Ce doping on improvement of luminescence performance for LaBr₃ crystals

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We investigated the band structure, electronic density of states and optical properties of lanthanum bromide (LaBr₃) and Ce-doped LaBr₃ ((LaBr₃:Ce) crystals using a first-principles calculation based on density functional theory (DFT). And the exchange correlation potentials among the electrons are described by using the generalized gradient approximation (GGA). Due to the transition of Ce³⁺ ion from 4f-orbital to 5d-orbital, the Fermi level of LaBr₃ crystal was changed after doping, with doping concentration of 4% is about 1.27 eV and 8% is about 1.05 eV. So the band gaps of LaBr₃:Ce (0.53 eV and 0.09 eV, respectively) is narrower than that of LaBr₃ (3.586 eV), which produce more visible light in the same range of irradiated energy. Otherwise, the absorption peaks (103482 cm⁻¹ and 156563 cm⁻¹, respectively) are smaller than LaBr₃ (203500 cm⁻¹), leading to transmit more visible light. Also, the reflection peaks of LaBr₃:Ce crystal are smaller than undoped LaBr₃ crystal in the range of visible light. The research shows reason that Ce doping can improve the luminescence performance of LaBr₃ scintillators and the results are compared with the available experimental data.

Thursday, 22/Aug/2019 12:12pm - 12:24pm

Abstract ID: 539 / FCM-3: 7

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Production and characterization of composite materials

Keywords: hybrid coatings, modified polyaniline particles, zinc, corrosion characterization

Hybrid Zn coatings with incorporated modified PANI particles – preparation and corrosion characterization

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Hybrid coatings based on polyaniline (PANI) improve the operating life of steel details against corrosion. In the present work, the preparation of stable suspensions of colloidal PANI-based particles, suitable for obtaining of composite anticorrosive coating on steel, is described. Electrokinetic data as a function of pH are presented, showing the correlation between the zeta potential of the PANI-based particles and the charged groups existing at the surface. Two types of PANI-based positively charged particles, suitable for electrophoretic deposition on steel (cathode) surface, are obtained: at pH 3.3 and after deposition of positively charged polymer molecules on negatively charged particles at pH 6.2.

Two types of PANI-based particles are prepared and thereafter incorporated during electrodeposition process into the metal matrix of zinc in order to obtain composite (hybrid) coatings. The latter are aimed to ensure sacrificial protection of steel mainly in aggressive media containing chlorine ions as corrosion activators which are leading generally to local corrosion damages. The surface morphology of the hybrid zinc coatings is investigated with SEM. The influence of PANI-based particles on the cathodic and anodic processes occurring in the starting electrolyte for obtaining of the zinc coatings is followed with cyclic voltammetry. The electrochemical and corrosion behavior is evaluated with Potentiodynamic polarization curves, Electrochemical impedance spectroscopy and Polarization resistance measurements. XPS and XRD studies are applied aiming to characterize the surface coatings appeared as a result of the corrosion treatment. The beneficial effect of the stabilized PANI-based particles for the increased protective ability of the composites is commented and discussed.

Wednesday, 21/Aug/2019 4:00pm - 4:12pm

Abstract ID: 540 / FBB-2: 1

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biomaterial surfaces

Keywords: surface functionalization, biofilm, infrared spectroscopy, in-situ monitoring

Bacterial development on functionalized surfaces: from first steps of adhesion to biofilm growth

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Bacterial adhesion to surfaces with subsequent development into closely associated populations (biofilms) is of great concern, particularly, in food industries and medicine fields. One strategy to prevent the development of pathogenic biofilms on abiotic surfaces is the use of probiotics (i.e. live microorganisms that when administered in adequate amounts confer a health benefit on the host). A biofilm of probiotic bacteria on the surface of interest may help to prevent attachment and proliferation of pathogenic species, similarly to as it happens in the human body. The control of the formation of biofilms requires the understanding of the initial step of the bacterial adhesion, which among others, is influenced by surface properties of the supporting material. Surface properties can be controlled via functionalization procedure with alkanethiol self-assembled monolayers (SAM) terminated with different functional groups. In this work, the formation of probiotic biofilms of *Lactobacillus Rhamnosus* GG (LGG) were monitored in-situ (directly in the nutritive medium) and in real time by means of infrared spectroscopy in attenuated total reflection mode (IR-ATR). Hydrophilic (-OH), hydrophobic (-CH₃) and positively charged (-NH₂) surfaces obtained by functionalizing IR-transparent ZnSe ATR crystal (nude or gold-coated), were used as support surfaces. Several methods were used to characterize modified ZnSe surfaces, including X-ray photoelectron spectroscopy, IR-ATR, atomic force microscopy, and contact angle measurements. Based on IR-ATR data and epifluorescence images recorded at the end of LGG inoculation period (2.5 hours), the process of bacterial attachment was affected by the choice of the surface function, which led to drastic differences in biofilm densities. Further maturation of LGG biofilms onto surfaces (24 hours) was not only surface-dependent, but also varied with respect to the choice of the nutritive medium. The relative content of nucleic acids, phospholipids, proteins and polysaccharides reflected the variation in metabolism of LGG in response to environmental changes. With this powerful physico-chemical approach, our data highlight the importance of surface interactions in the development of biofilms of LGG on abiotic surfaces.

Abstract ID: 541

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Advances in the Synthesis and Characterization of low dimensional, nano and 2D materials

Keywords: Layered crystals, piezoelectric properties, ultrasonic method

Two-dimensional CuInP2S6 family crystals and their applications for piezoelectric transducers

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Two-dimensional CuInP2S6 family crystals and their applications for piezoelectric transducers

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The interest in (2D) ferroelectrics is motivated by the prospect of using their piezoelectric, ferroelectric, electromechanical and dielectric functionalities for applications of high performance functional electronics. A promising family for this type of development is the crystals of layered phosphorous chalcogenide SnP2S6, CuInP2S6 and their derivatives [1, 2]. These crystals possess figures of merit for piezoelectric properties comparable to that of widely used piezoelectric materials. The phase transition temperature of CuInP2S6 could be raised till 340K what it is important for applications. SnP2S6 crystals are piezoelectric till melting temperature. In this contribution we present experimental studies of ultrasonic and piezoelectric properties in SnP2S6, CuInP2S6 crystals. The high frequency ultrasonic method was used for investigations of piezoelectric sensitivity. The measurements of ultrasonically detected piezovoltage in the ferroelectric phase were used for the characterization of ferroelectric switching in DC field and the developing of polar state in CuInP2S6 samples. The piezoelectric sensitivity due to electrostriction could be induced in the paraelectric phase of CuInP2S6, or in nonpolar AgInP2S6 layered crystal. In this case DC bias electric field was applied along the polar direction perpendicular to layers. In investigated (2D) CuInP2S6 family crystals at room temperature electro-mechanical coupling for thickness vibrations as high as 50 % could be obtained, after appropriate poling [2, 3]. This is important for medical diagnostics ultrasonic transducers applications.

Key Words: Layered crystals, piezoelectric properties, ultrasonic method

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Thursday, 22/Aug/2019 3:42pm - 3:54pm

Abstract ID: 542 / FCM-4: 9

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: magnetic polymer NCPs; Tween 80; emulsion polymerization; encapsulation efficiency; monomer conversion

Tailoring emulsion polymerization for high-yield synthesis of Tween 80 stabilized magnetic polystyrene nanocomposite particles

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Tween 80 coated magnetic polymer nanocomposite particles (NCPs), as functional materials with good biological application prospect, still suffer from a challenge to efficiently yield the desired products without plain polymer particles and aggregation of particles. In this study, Tween 80 coated NCPs were synthesized using seeded emulsion polymerization, which solely stabilized by Tween 80 and initiated by oil-soluble initiator, 2,2'-azobisisobutyronitrile. The effects of Fe₃O₄, monomer, initiator and emulsifier dosages on the monomer conversion, encapsulation efficiency and particle characteristics were investigated, among which the Tween 80 dosage was found to be the key factor for high-yield synthesis of desired NCPs. Through a precise control over Tween 80 concentration in colloidal Fe₃O₄ clusters using a micro-mixing method, monodispersed NCPs with high monomer conversion of 70.1 % and high encapsulation efficiency of 100 % were successfully obtained after a duration of 3.5 h. The mechanism to achieve controlled NCPs synthesis was also revealed by figuring out the time profiles of monomer conversion and products morphology during the course of NCPs preparation.

Abstract ID: 543

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Fundamental investigations on low-dimensional nanomaterials and their functional structures properties

Keywords: Graphene Fiber, Direct Fabrication, Multi-level, Functional Device, Assemblies

The In-situ fabrication of multi-level graphene fiber and its applications

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With the fast development of wearable technology, functional materials and devices have been attracting more and more people's attentions in many fields. The next generation wearable devices require novel materials with excellent mechanical flexibility, light weight and ease for textiles. Graphene fibers, assembled from graphene sheets, have versatile promised applications such as functional textiles, photoelectrodes, flexible and wearable devices, etc. However, the traditional wet-spinning technology of graphene fiber still has some disadvantages, such as poor maneuverability and difficult to further process, which greatly limit its application in many fields. Here, we report the direct fabrication of different kinds of graphene fiber assemblies, such as multi-ply fibers, spiral fibers, core-sheath fibers and networks, by modulating the wet-spun process and the movement, structures and numbers of the spinnerets. Remarkably, we explored the relationship between structure and performance of these kinds of graphene fiber assemblies. Such graphene fiber assemblies present excellent stretch and electric properties due to their unique structures, which can be used in sensors, supercapacitors and batteries. Moreover, our assembly strategy provides a new insight into the construction of integrated high-performance graphene fibers for multifunctional applications and purpose in the future.

Abstract ID: 544

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Magnetic Nanomaterials for Applications

Keywords: Magnetic Nanostructures, Silicon, Ion Implantation

Enhanced room-temperature magnetoresistance of metal/silicon/metal junctions with embedded nickel nanostructures formed by ion implantation

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Integration of magnetic functionalities with silicon for efficient generation of spin-polarized carriers in this dominant semiconductor material under operational conditions remains a great challenge. Here we report an approach to the synthesis of ferromagnetic nanostructures embedded within a silicon crystal. This involves the use of hydrogen ion implantation for creation of nanoscale voids in the Si crystal followed by the gettering of surface implanted nickel atoms to the nanocavities. The resultant embedded Ni nanoparticles have size 10-30 nm and density $\sim 1E10/cm^2$, and their immediate surroundings are in a very high crystalline quality. Ni nanoparticles encapsulated within such high-quality crystalline Si exhibit a large magnetic moment on the order of 1500 μB , enabling strong room temperature ferromagnetism with a high magnetic switching energy barrier of ~ 0.86 eV. Metal/silicon/metal junctions with embedded nickel nanostructures show enhanced positive magnetoresistance for both p- and n-Si at room temperature. A spin-split band model is used to explain the magnetoresistance behaviors and relevant parameters such as spin-splitting and g-factors for the Ni nanostructured layer are determined. From this model, spin polarization at room temperature is estimated to be above 90% for both p-type and n-type Si with embedded Ni nanostructures. These results suggest that our approach based on ion implantation and metal gettering at nanocavities could be promising in creating novel Si material structures and devices for spintronic applications.

Abstract ID: 545

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Polymeric composites

Keywords: Silica Aerogel, PS/Silica Nanofibers, Electrospinning, Thermal Insulation

PS/Silica Aerogel Nanofibers Production for Thermal Insulation

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Aerogels are fascinating solid materials made up with over 95% air and less than 5% skeletons [1]. With the advantages of an extremely low density of 0.003–0.5 g/cm³, a low thermal conductivity of 0.017–0.021W/m·K and a high specific surface area of 500–1200 m²/g [1–3], aerogels have enormous application potential in various fields, such as thermal insulators, energy conservation, catalyst supports, biomedical engineering and aerospace applications [3–9].

In this work, silica aerogels were synthesized as stated by Li et al. [10]. Commercial polystyrene (PS) was used instead of polymerization of styrene monomers to obtain PS/silica aerogels nanocomposites. Furthermore, nanofiber structure was obtained by electrospinning. The specific surface area, pore volume and particle size of aerogels, which are 590 m²/g, 1.4 cm³/g and 10 nm, respectively, were determined by BET analysis. Thermal gravimetric analysis indicated that the maximum degradation temperature of PS shifted from 412 to 444 °C when silica aerogels content at 10wt%. Regards to improvement in thermal stability, PS/silica aerogels nanocomposites can be a promising candidate for thermal insulation applications.

Abstract ID: 546

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Particulate reinforced Composites

Keywords: Elasticity, Elastic properties, Spherical nanocomposites, Particulate composites

On Hashin's bounds for elastic properties of spherical particle-reinforced composites with graded interphase

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Macroscopic properties of particle-reinforced composite materials are strongly influenced by the phenomena at the interface between particles and the matrix. The paper is focused on analytical prediction of the effective bulk and shear modulus for particulate composites reinforced with solid spherical particles surrounded by graded interphase zone. A three-dimensional elasticity problem for a single inclusion embedded in a finite matrix is studied. The graded interphase zone around the inclusion is assumed to have power law variation of the shear modulus with radial co-ordinate, with Poisson's ratio assumed to be constant and equal to that of the matrix. Following Hashin's approach, two boundary value problems are considered and stress and displacement fields in the interphase zone are determined. They are then used to calculate the elastic energy for the single inclusion composite under spherically symmetric state and pure shear state and derive closed-form expressions for the bulk modulus and the upper and lower bounds for the shear modulus. Numerical results for hard and soft interphase zones are presented and discussed for a range of the interphase zone thickness ratios. The interphase zone permits us to increase the properties of nanocomposites and the parametric investigations of this study furnish useful information in the design phases of nanocomposites.

Abstract ID: 547

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Invited Talk

Topics: Applications of Biopolymer for Drug Delivery

Keywords: Sodium alginate, Hydrophobic modification, Nanoparticles, Drug delivery

Alginate-based micro/nanoparticles for the delivery of drugs

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Sodium alginate (SA), an anionic polysaccharide with good biocompatibility, can form hydrogel by chelating with divalent cations such as calcium ion. The calcium alginate hydrogels have been used to entrap cells for transplantation or drugs for sustained release [1,2]. However, the hydrophilic property and three-dimensional network with larger pore size of alginate hydrogel are against the entrapment of both hydrophilic drugs (such as peptides and proteins) and hydrophobic drugs. Burst release of hydrophilic drugs or impossible diffusion of hydrophobic drugs always results in subsequent poor bioavailability [3].

To improve the release behavior of drugs, the modification of sodium alginate has been carried out [4], such as hydrophobic graft or coating with other polymers. Here, SA was hydrophobically modified with vinyl acetate (VA) by graft copolymerization. FTIR spectra displayed the stretching vibration peak of carbonyl group at 1751 cm⁻¹ evidenced the grafting of VA on hydroxyl group of alginate to give the hydrophobic side chain. The degree of substitute (DS) can be controlled as low as 20% so that the product could still keep hydrophilic backbone but graft hydrophobic side chain. SA-g-PVAc can be dissolved in water and sequentially be prepared as novel calcium-SA-g-PVAc hydrogel micro- or nano- particles through gelation or ultrasonic self-assembly, which showed comparable properties (e.g. size and mechanical strength) with the hydrophilic alginate hydrogels. The diffusion evaluation with different molecules demonstrated that calcium-SA-g-PVAc microparticles hardly had resistance to small hydrophilic molecules. While the hydrophobic modification not only facilitated the release of water-insoluble small anticancer drugs, but also improved the entrapment and release of proteins from the novel hydrophobically modified alginate micro- or nano- particles.

Abstract ID: 548

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalysis and Energy

Keywords: graphene oxide, molecular metal complex, hydrogen photoproduction

Reduced Graphene Oxide Immobilized with Pyrene-pendant Rhodium Catalyst and Platinum

Nanoparticles: Enhanced Hydrogen Photoproduction

Reduced Graphene Oxide Immobilized with Pyrene-pendant Rhodium Catalyst and Platinum Nanoparticles: Enhanced Hydrogen Photoproduction

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A cyclopentadienyl rhodium catalyst derivatized with pyrene was used to study the effects of a reduced graphene oxide (rGO) on visible light-driven photocatalytic hydrogen production using formate and Pt nanoparticles. The pyrene-derivatized rhodium catalyst was immobilized on rGO by π - π stacking interactions. A tight formation of the Rh catalyst on rGO surprisingly enhanced the hydrogen production upon visible light irradiation, in contrast with the results using a thin formation of the catalyst or the unfunctionalized Rh catalyst. Our results also demonstrated that the catalytic stability of the pyrene-functionalized Rh complex dramatically increased when it was immobilized on rGO during the photocatalytic reaction cycle. RGO played a crucial role in efficiently transferring electrons from the Rh(III)-hydrides to the platinum nanoparticles. In this study, we report the visible light-driven photoproduction of hydrogen using a pyrene-derivatized rhodium complex anchored on rGO by π - π stacking interactions. First, we show a surprising enhancement effect of rGO on hydrogen photoproduction with the molecular rhodium catalyst and formate in the presence of PtNPs upon visible light irradiation in an aqueous solution. The production rate was dependent on the density of the Rh catalyst on rGO. In addition, evidence is presented that supports the much higher stability of the Rh catalyst immobilized on rGO during photocatalytic hydrogen production.

Abstract ID: 549

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Piezo-phototronics for energy science and optoelectronics

Keywords: ZnO, Bent strain, Atomic-bond-relaxation, Piezoelectric properties

Curvature-dependent band engineering and piezoelectric properties in bent ZnO nanowires

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Curvature-dependent band engineering and piezoelectric properties in bent ZnO nanowires

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It has long been challenge regarding the atomic-level mechanism of how mechanical deformation can modulate band structures as well as polarization and piezoelectric properties in bent ZnO nanowires (NWs). Moreover, a theoretical relationship among the band shift, polarization and bond identities of ZnO NWs is still lacking. Here, we investigated the coupling effect of bending curvature and nanowire size on the band offset and nonlinear piezoelectric properties of ZnO NWs based on the atomic-bond-relaxation (ABR) correlation mechanism and continuum medium mechanics. We found that the mean bond length of ZnO NWs elongates with decreasing radius of curvature and the bandgap decreases non-linearly with increasing curvature. Also, the piezoelectric constant increases with decreasing diameter of ZnO NWs, which provides a better understanding of the red-shift of bandgap and the increased piezoelectric voltage output with increasing curvature as well as the related size effect.

Key Words: ZnO, Bent strain, Atomic-bond-relaxation, Piezoelectric properties

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Wednesday, 21/Aug/2019 6:15pm - 6:27pm

Abstract ID: 550 / FC: 12

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Photocatalysis

Keywords: Photocatalysis, Hydrogen production, Heterostructure

Promoting efficient spatial charge separation and transfer for enhanced photocatalytic hydrogen production from water splitting

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Environmental pollution and energy shortage are the major challenge which humanity is facing today. Photocatalytic hydrogen evolution from water splitting, which directly converts solar energy into clean chemical energy without pollution, has attracted much attention. Heterostructures consisting of two or several semiconductors present a promising perspective due to the fact that heterostructures are very beneficial to the separation and migration of photogenerated charge carriers. In recent years, our group has devoted to improving photocatalytic hydrogen production performance by promoting efficient spatial charge separation and transfer. We developed a series of heterostructures, such as CdS@ZnO core-shell structure, CdS quantum dots/ZnO nanosheets 0D/2D heterojunction, g-C₃N₄/C-TiO₂ hollow structures, In₂S₃/CdIn₂S₄/In₂O₃, etc. Our results showed that the photocatalytic hydrogen production was significantly enhanced due to the efficient spatial charge separation and transfer.

Key Words: Photocatalysis, Hydrogen production, Heterostructure, Z scheme

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Abstract ID: 552

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Metal matrix composites

Keywords: W-Mo-Cu composites, electric current, rapid sintering, densification

Study on the effect of electric current on the W-Mo-Cu composites rapidly prepared by large current electric field sintering

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The novel W-Mo-Cu composites, combining the advantages of W-Cu and Mo-Cu composites, was rapidly prepared by large current electric field sintering performed by Gleeble thermo-mechanical simulator at a low temperature (975 °C) in a short time (5 min). Electric current (30,000-50,000A) effects on the sintering process, microstructure and properties of W-Mo-Cu composites were comprehensively studied. The comprehensive analysis of XRD and TEM show that W-Mo-Cu composites consist of W, Mo, Cu phase and a new phase of Cu_{0.4}W_{0.6} intermetallic compound, indicating that the large current as the heat source can induce Cu atoms to enter into W crystal to produce intermetallic compound during the sintering process. The calculated densification activation energy shows a decreasing trend with the increase of electric current, accelerating the diffusion among atoms, which is conducive to the sintering densification. With increasing electric current, the size and number of sintering necks increase and a microstructure with less and smaller pores is obtained, leading to a remarkable increase in relative density from 84.51% to 98.74%. Moreover, the micro-hardness increases and the electrical resistivity decreases. This study provides suggestive insights for the further development of the preparation of W-Mo-Cu composites by large current electric field sintering.

Abstract ID: 553

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Particulate reinforced Composites

Keywords: silica-gel nanocomposite, enhanced mechanical property, spectral properties

Nanoparticles Reinforced Silica Gels: Structure and Properties

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It draws many researchers' interest to incorporate nanoparticles into various materials matrix (polymers, metals and ceramics, etc.) to enhance their performance. In this paper, a comprehensive research has been conducted for the sol-gel process to prepare various nanoparticle-doped silica glasses to study how different nanoparticles changed the physical properties of the composites and their possible forming mechanisms. The nanoparticles used were oxides (TiO₂ (5 nm), Al₂O₃ (25 nm), ZrO₂ (50 nm)), carbides (B₄C (50 nm), WC (50 nm), TiC (50nm), SiC (50 nm)) and carbon allotropes (graphene (1-5 nm), and MWNT (10-30 nm)). The effect of the nature and size of nanoparticles on the mechanical and spectral property of the nanocomposites was studied. The result shows that oxide nanoparticles disperse better. The smaller the nanoparticles are, the better the dispersion. It can be confirmed by using both HRTEM (EDS) and FT-IR that the oxide nanoparticles modify the glass structure by interacting with water molecules and hydroxyl groups during sol-gel process and resulting in order, denser and three dimensional gel products. Coarsening of the microstructure and the strengthening of the gel network enhance the hardness and flexibility of the gel. The nanoparticles provide a good and solid support for the immobilization of other functional materials like electrical, optical and thermal sensitive substances. The absorption and emission spectra of the nanoparticles reinforced silica gels show the advantages of the nanoparticle addition and they have great potentials to be used in the development of pH, metal ions or organic gases sensing products.

Abstract ID: 554

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Alloy anodes

Keywords: Dealloying; Bimodal pore; β -CuZnAl shape memory alloy; Current collector; Li ion battery

A novel 3D submicro-nano bimodal porous β -CuZnAl shape memory alloy current collector for binder-free lithium ion batteries

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Sn anode is considered to be one of the most promising anode materials for new-generation lithium ion batteries with high capacity and energy density. However, Sn anodes suffer from huge volume change during cycling, which would lead to the sharply decreased capacity. Conducting bimodal porous metal as current collector was thought to an efficient way to accommodate the volume expansion of Sn anode. However, the long cycling life still cannot be achieved for the ligaments of the pores are too soft to endure the large volume expansion of Sn, which would cause severe plastic deformation or collapse of porous structure. In this study, the ligaments of the bimodal pores were enhanced by conducting β -CuZnAl shape memory alloys (SMAs) with high recovery ability by one-step dealloying of Cu-34Zn-6Al (wt.%) precursor and subsequent vacuum heat-treatment. After electroless plating of Sn, the Sn electrode with bimodal porous β -CuZnAl SMAs current collector shows a more stable cycling performance and higher areal capacity than the Sn electrode with planar copper foil and another Sn electrode with bimodal porous current collector without super-elasticity. It could be expected that this novel bimodal porous β -CuZnAl SMAs current collector also can be of great use in other types of metal-based anodes with high specific capacity, which also suffer from huge volume expansion.

Abstract ID: 555

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Composite structural materials

Keywords: Magnesium oxychloride cement, basalt fiber, Mechanical Properties thermal stability

Mechanical Properties and Thermal Stability of Basalt Fiber Reinforced Magnesium Oxychloride Cement

Xiang Li, Yuan Zhou, Chunxi Hai, Xiufeng Ren, Jinbo Zeng, Yue Shen, Yanxia Sun

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Magnesium oxychloride cement (MOC) has many advantages such as light weight, high strength, and low thermal conductivity which has drawn attention in the field of building energy conservation as an inorganic heat preservation and insulation materials in recent years. However, due to the poor high and low temperature mechanical property, as well as highly brittle behavior, limit its applications. In this study, chopped basalt fiber with different fiber contents by mixture volume (i.e. 0–1 %) and lengths (i.e. 10 mm–20 mm) were added into MOC matrix. The effect of chopped basalt fiber on the compressive, flexural, and splitting tensile strengths as well as the effect of different temperatures (up to 300 °C) on the strength of fiber reinforced MOC were investigated and the longitudinal wave velocity and wave form were studied by ultrasonic testing. Meanwhile, the fracture surface and morphology of specimens were performed by SEM. The results of test showed use of chopped basalt fibers had little effect on the concrete compressive strength; however, significantly improved the flexural, and splitting tensile strengths as well as the thermal stability of MOC.

Abstract ID: 556

Symposium 6: Functional Thin Films (FTF)

Plenary

Topics: Micro/Nano-electronics and MEMS

Keywords: smart materials, shape memory alloys, thin film, NiTi

NiTi thin film shape memory alloys: A Smart Materials

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With emerging technological advances, the industrial highlight and extensive research on smart materials. Shape memory alloys (SMAs) belong to a class of shape memory materials, which have the ability to 'memorise' or retain their previous form when subjected to a certain stimulus such as thermomechanical or magnetic variations etc. SMAs have drawn significant attention and interest in this progressive year in a broad range of commercial applications, due to their unique and superior properties; this commercial development has been supported by fundamental and applied research studies. This presentation describes the attributes of NiTi SMAs which will be used in Micro-mechanical systems and addresses their associated limitations to clarify the design challenges faced by SMA developers. An extensive discussion on sputtered NiTi deposition on Silicon substrate will be discussed.

Abstract ID: 557

Symposium 6: Functional Thin Films (FTF)

Invited Talk

Topics: Thin films for optoelectronics, nanoelectronics and spintronics

Keywords: Flexible Electronics, Printed Electronics, Printing Techniques, Organic Electronics

Printable Conductive Thin Films for Flexible Electronics

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Flexible and stretchable electronics represent today's cutting-edge electronics. Printing techniques are an important enabling technology for the development of low-cost, large-area, and flexible optoelectronic devices. Conductive thin films made from solution-processable transparent conductive materials, such as metal nanoparticles/nanowires, carbon nanotubes, graphene, and conductive polymers, can simultaneously exhibit high mechanical flexibility, low cost, and better photoelectric properties. This is an area where novel materials combined with novel device fabrication process hold great promise. Our approach in addressing this interesting field is to develop new materials with promising optoelectronic performance at a low price and to try novel device fabrication methods such as inkjet printing. The room temperature solution processing we adopt enables easy synthesis of electrode materials that holds great promise for mass production. The use of printing methods not only lowers the device fabrication cost, but also enables novel device structure, resulting in devices better suitable to the requirements of flexible devices.

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Abstract ID: 558 / Poster: 37

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Nanomaterials for Sensors, Flexible Electronics and Nanocomposites

Keywords: Graphene; Microstructures; Dielectrophoretic force; Microdevice

Detecting Heavy Metal Ions by Graphene Flakes-Based Microdevices

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We propose to detect copper and palladium ions with ultra-low concentrations by a microdevice integrated with microelectrode array. The microdevice was fabricated by parallel assembly of individual graphene flakes into microstructures via dielectrophoretic force. The microstructures dielectrophoretically assembled by graphene flakes can bridge the 2- μm gap between the two facing microelectrodes, which allows the assembled graphene microstructures with low impedance to be electrically characterized. The impedance of assembled microstructures was changed when the external ions were adsorbed on graphene in the experiment. It also leads to difference in electrical characteristics of the microstructures such as current-time (I-t) characteristics or cyclic voltammetry (C-V) when different types of ions were applied. This graphene-electrode structure is sensitive to the ultra-low concentration ($< 3 \text{ pM}$) of the ions (Cu^{2+} and Pd^{2+}) which are the heavy metal ions and harmful to human health. This study experimentally demonstrates the feasibility for a sensitive method in the application for detecting heavy metal ions with ultralow concentrations.

Abstract ID: 559

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Intelligent biomaterials

Keywords: Temperature, influence, hydrogels, self-healing, high stretchable

Preparation temperature influence on the properties of hydrogels

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Man-made materials with self-healing capabilities are highly desirable and their development has become a goal for many scientists and engineers.¹⁻⁴ Generally, properties of materials are difficult to change unless with the help of the incorporation of new functional groups. Herein, we found that the 2-hydroxyethyl methacrylate and acrylamide (HEMA/AAM) hydrogels can be easily reversed from non-self-healing to rapidly self-healing by simply changing the reaction temperature. Interestingly, the hydrogels that are prepared at room temperature do not exhibit self-healing behavior, while those treated at an elevated temperature can show self-healing performance healing performance within only ~15 s. Different compared with the previous self-healing polymer HEMA hydrogels that function only above their glass transition temperatures (T_g), these hydrogels exhibit self-healing properties at room temperature, which is lower than the T_g of the hydrogels. In addition, the stretching capabilities of the hydrogels can be greatly increased by up to 30-fold. The hydrogels also showed good adhesive performance and they adhered strongly onto wood, glass, and steel. These results would have great influence on the design of self-healing hydrogels and their large-scale production.

Abstract ID: 560

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Polymeric composites

Keywords: Anti-Crude-Oil-Adhesion, Amphiphobic Coatings, Amphiphilic Coatings, Liquid Repellency

Coatings with crude oil repellency

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Current petroleum refining technologies have focused on the modification of crude oil composites to decrease their adhesion and thus facilitate oil extraction, transportation, storage, and processing. Existed methods such as heating, dilution, emulsification, or the addition of substances that can reduce drag inside pipelines are energy-intensive and suffer from various limitations.¹⁻³ Herein, we present a conceptually different waterborne coating strategy to eliminate these drawbacks. The novel crude oil-repellent coating was designed and prepared by crosslinking the polymer particles and silicone surfactant that bearing hydroxyl groups with the melamine formaldehyde resin in a green and industrially-viable process. Considering the unique anti-crude-oil-adhesion properties, the wide range of applicable substrates, and the outstanding physical and chemical stability, we expect that this coating can provide a promising starting point toward the functionalization of the surfaces of instruments or pipelines that are otherwise prone to the adhesion of crude oils.

Abstract ID: 561 / Poster: 24

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Biomaterial surfaces

Keywords: Biomaterials, femtosecond laser processing, functional surface, biopolymers, bioceramics, tissue engineering

Controllable patterning designs of biomimetic thin film coatings induced by femtosecond laser texturing for cellular guidance

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Biomaterials for bone tissue engineering applications should possess excellent bioresorbability and bioactivity characteristics. The achievement of stable surface contact between the bone tissue and implant surface is a critical requirement for the development of ideal scaffolds. Combining the osteogenic properties of natural polymers with good mechanical properties of ceramic biomaterials, substitutes for bone regeneration with improved surface properties can be designed [1, 2]. Chitosan is one of the most widely accepted biodegradable and biocompatible natural polymers. Hydroxyapatite (HAp) is the main component of bone tissue. Its incorporation to the composite layer contributes to cellular affinity and will improve the ingrowth of bone cells. Zirconia (ZrO₂) insertion will contribute to achieving enhanced mechanical properties of the interface layer. We synthesize thin chitosan (CH) /Hydroxyapatite (HAp)/ ZrO₂ composite thin films with different ratios and evaluated their characteristics. The goal of the present study was to investigate the possibility of applying femtosecond laser surface texturing (LST) to modulate surface characteristics of widely used in bioengineering naturally derived polymer/ceramic biofilms. Via tuning of laser irradiation parameters, diverse structure morphology (shape, size, and porosity) of thin biofilms surface can be achieved. The laser treatments were carried out by applying direct laser patterning. We textured the biofilm surface with quadratic, triangular and stripe-like shapes by means of laser photomodification using a Ti: sapphire femtosecond laser focused onto the specimen surface. Selection of a set of laser processing parameters, permit the recognition of different patterning regimes leading to unique surface morphologies (porous microfoam).

The prepared interface layers were characterized using SEM, EDX, FTIR, and XRD. MC3T3 cellular viability and attachment were evaluated on the textured composite layers and demonstrated geometrically ordered cellular networks.

Abstract ID: 562

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Polymeric composites

Keywords: Epoxy Polymer, Branched Amine, Composites

The Synthesis of Branched Amines with polyether and the Studies of Physical Properties of Epoxy Composites Including the Amines

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Epoxy polymers have been interested in industries for the purpose of composites, coatings, or adhesives. The epoxy resin forms polymer networks by reacting with curing agents such as amine derivatives, acid anhydrides, or amide derivatives. The epoxy curer can be divided into two categories. One is a liquid curing agent proceeding polymerization at room temperature. The other one is a solid type of curer initiating chemical reaction with epoxy resin under the specific thermal energy. For the room temperature reaction, there are a lot of amine compounds such as ethylene diamine, triethylenetetramine, tetraethylenepentamine, or isophorone diamine to form epoxy polymers.

These amine compounds are excellent in reactivity with epoxy groups, but the cured polymer tends to undergo crack propagation due to brittleness under external impacts. Therefore, various toughening agents such as core/shell particles, or polyurethanes are developed to compensate for the issue. The other methods to enhance impact resistance of the polymers are using flexible amine curers. While there are numerous flexible amine compounds or polymers, Jeffamine D-230 or D-400 is one of representative flexible diamine curer composed with ethylene oxide repeating unit.

In this report, we first prepared ethylene tetraacrylate (ETA) by reacting ethylene diamine with acrylate with 1:4 molar ratios. After that, 4 equivalent of Jeffamine D-230 or Jeffamine D-400 was reacted to ETA to form final products (JP-2 from Jeffamine D-230 reactant, JP-4 from Jeffamine D-400), respectively. The prepared different amount of amine derivatives were respectively added into epoxy compositions composed with bisphenol A epoxy resin and Jeffamine D-230 curer. The prepared epoxy compositions were cured in an oven at 100 °C to obtain epoxy polymers. The changes of mechanical properties of the prepared polymers were studied by performing the measurement of flexural and impact strength. The obtained results suggest that the prepared amine compounds provide excellent impacted resistance with the small amount of addition of JP-2 or JP-4.

Abstract ID: 563

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Homogeneous and Heterogeneous Catalysis

Keywords: Polymeric acidic ionic liquids, acetalation, polyoxymethylene dimethyl ethers

Novel polymeric acidic ionic liquids as catalysts for the preparation of polyoxymethylene dimethyl ethers

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Polymeric acidic ionic liquids (PAILs), which combine the desired catalytic properties of ILs and polymer feature of insolubility in commonly used organic solvents, have been investigated extensively in several recent studies. The concentration of AILs on the surface of PAILs is higher compared with other supported AILs. The most common type of PAILs are those bearing pendant AILs and acid groups in a polymer chain, prepared from the polymerization of an AILs monomer or a precursor, including imidazolium –SO₃H heteropolyanion, poly(4-vinylpyridine), copolymerization of AILs oligomers with divinylbenzene (DVB), copolymerization of AILs oligomers and resorcinol-FA (RF resin), and polymerization of 2-acrylamido-2-methyl-1-propanesulfonic acid with butylamine or 2-(N,N-dimethylamino) ethyl methacrylate. Most of the reported PAILs possessed carbon-carbon double bond polymerization on the cations, while the anions bonded with cations only by ionic bonds. Since the acid sites on the surface fell off easily, the catalytic activity decreased more or less during reuse and hence the stabilities of these catalysts need to be improved.

A series of mesoporous and macroporous polymeric acidic ionic liquids (PAILs) have been successfully synthesized and subsequently characterized using Fourier transform-infrared spectroscopy, N₂ adsorption-desorption isotherms, scanning electron microscopy and thermogravimetry. Furthermore, the catalytic performance of the synthesized PAILs was investigated for the acetalation of methylal (DMM1) with 1,3,5-trioxane (TOX), mesoporous and macroporous PAILs copolymerized by both cations and anions exhibited moderate to excellent catalytic activities for the acetalation. Moreover, the influence of various reaction parameters was investigated by employing [polyVPyBs]_p-SsO(rt.) as the catalyst and it demonstrated high thermal stability and excellent reusability.

Abstract ID: 564

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Green catalysis

Keywords: basic ionic liquids, nitrogen-bearing heterocyclic group, CO₂

New functionalized ionic liquids derived from nitrogen-bearing heterocyclic compounds

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The most attractive characteristic of ionic liquids is their designability. By attaching specific organofunctional group to the structure of ionic liquids, they can be used as reactions medium, catalysts, functional materials, and so on. Recently, basic ionic liquids containing basic group in cation or anion were found to be environmental-friendly solvents and catalysts with high activity and selectivity and easily recovered materials, which have the potential to replace traditional bases such as KOH, NaOH, triethylamine, or tetrabutylammonium acetate.

Herein, we designed a series of base-functionalized ionic liquids by incorporating nitrogen-bearing heterocyclic group in the structure. In order to obtain the relationship between structure and alkalinity, DFT and potential titration were carried out. With these new ionic liquids in hand, we also investigated their catalytic performance in activation and conversion of CO₂.

Thursday, 22/Aug/2019 3:03pm - 3:15pm

Abstract ID: 565 / FCM-4: 6

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: ZIF-67, GO@ZIF-67, adsorption, photocatalytic, methylene blue, methyl orange

PHOTODEGRADATION OF ORGANIC DYES USING COBALT-BASED METAL ORGANIC FRAMEWORK (ZIF-67) CATALYSTS SUPPORTED ON GRAPHENE OXIDE UNDER SIMULATED SOLAR IRRADIATION

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The photocatalytic degradation of methylene blue and methyl orange was achieved under solar light simulated conditions using Zeolitic imidazolate framework-67 (ZIF-67) anchored on graphene oxide (GO) sheets. The composition, structure and morphology of both the self-standing ZIF-67 and the graphene oxide supported analogue, GO@ZIF-67 composites, were analysed and confirmed using a variety of techniques such as FTIR, BET, SEM, TEM and Zeta potential. The ZIF-67 frameworks structures retained their crystallinity (octahedrals of 300 – 500 nm size) even when supported on GO sheets. ZIF-67 crystals had a high specific surface area ca. 1185.1 m² g⁻¹ with a pore volume of 0.0069 m³ g⁻¹ and the pore diameter of 2.6 nm. The GO@ZIF-67 composites exhibited high adsorption for methylene blue (MB) compared to that of methyl orange (MO). The maximum adsorption capacity reached up to 220.00 mg g⁻¹ within 2 h for MO. Further catalytic degradation of the same dyes (MB and MO) showed that degradation efficiency was quantitative for MB and reached a maximum for MO. The GO@ZIF-67(0.1) composites proved to be the best photocatalyst for MB as compared to the rest of the combinations. The kinetics of the adsorption and photocatalytic processes will be presented and related to the nature of the dyes, i.e. cationic versus anionic.

Abstract ID: 566

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Nanostructured materials for advanced batteries

Keywords: carbon, porous, doping, oxygen reduction reaction

Insight into the Synergistic Effect between C-S and Fe-N Sites for Oxygen Reduction Reaction in Alkaline and Acidic Media

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Developing nonprecious metal electrocatalysts with excellent ORR performance and superior stability in both alkaline and acidic media is always being a challenge. Herein, we successfully prepared Fe, N, S co-doping porous carbon nanosheets by means of simply pyrolyzing low-cost carbon precursors, which exhibited superior ORR activity and stability in both alkaline and acidic media. The thin porous carbon nanosheets with a twisted morphology and distorted graphene layers possess abundant carbon defects and highly dispersed active sites, which contribute to the improved ORR activity. By precisely controlling the content matching of C-S and Fe-N sites, we discovered that the synergistic effect between C-S and Fe-N sites could be maximized only when they reached the balance, so that the catalyst exhibited the optimal ORR activity. And the synergistic effect is more conspicuous in acidic media. Compared with the current complicated preparation process, the simple approach we adopted has overwhelming advantages. It is meaningful to conduct the quantitative research of active sites to optimize catalysts and maximize the ORR activity. Our research provides a new idea for the development of Fe, N, S co-doping ORR electrocatalysts in the future.

Abstract ID: 567

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Composite structural materials

Keywords: local clay, thermal activation, metakaoline, disorderness, geopolymer

oral presentation

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Thermal activation of local clay at Khyberpakhtunkhwa, Pakistan for the production of geopolymer at low cost

Abstract

The present study involves the thermochemical treatment of locally available clay at Khyber Pakhtunkhwa Pakistan and to utilize in the synthesis of geopolymer as a binding material. The clay activated at 500, 600, 700, 800 and 900oC was used in the synthesis of geopolymer. The structural and morphological changes in the clay with thermal treatment and that of geopolymer were studied using X-Ray diffraction (XRD), Fourier transform infrared (FTIR). The results demonstrate that the thermal treatment of clay at 900oC is more effective which convert kaolinite into meta-kaolinite and give good quality geopolymer.

Key words: local clay, thermal activation, metakaoline, disorderness, geopolymer

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Abstract ID: 568

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Structural, Electronic, Optical and Magnetic Properties

Keywords: CsI(Tl) crystal; Luminescence decay time; Crystal size; Emission spectrum; X-ray excitation

Effect of crystal size on luminescence properties of CsI(Tl) crystal under X-ray excitation

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The bulk CsI(Tl) crystal's applications for computed tomography (CT) and other high-speed imaging has been hindered by its relative slow scintillation decay afterglow. We manufactured nanometer, micrometer and millimeter scale of CsI(Tl) crystals, and measured the luminescence decay time of bulk CsI(Tl) crystals and three scales CsI(Tl) crystals under sub-nanosecond intensive pulsed X-ray excitation. We found out that the bulk CsI(Tl) crystals presented a slow decay time component $3.2 \pm 0.07 \mu\text{s}$ and a fast decay time component $736 \pm 2.6 \text{ns}$. But when the CsI(Tl) crystal diameter decreased to millimeter-scale, its X-ray excited luminescence decay time mainly centralized in about 1000 ns, and their 5 keV cathode luminescence peak and 235 nm photon excitation luminescence peak were all at 540 nm. In addition, the emission spectra of these three scales CsI(Tl) crystals under 235 nm photon excitation show that the smaller scale CsI(Tl) crystals emit more intense luminescence because they have higher light absorption (235nm) – emission(540 nm) efficiency which were confirmed by the 235nm excitation spectra results. These experiment results suggests that the CsI(Tl) crystal size reduction influences its X-ray luminescence decay property and 235 nm excitation luminescence. Such a property makes CsI(Tl) crystals a potential material for certain detectors that required no afterglow scintillators.

Thursday, 22/Aug/2019 2:27pm - 2:39pm

Abstract ID: 569 / FCM-4: 3

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Polymeric composites

Keywords: Rare earth Doped Nanoparticles, Photonic Composites, Optical Waveguides

Infrared Emitting Photonic Composites for Polymeric Waveguide Amplification

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Amplification of optical fields is a fundamental function needed in the processing of optical signals for photonic devices. On-chip waveguide amplifiers offer higher gain in small device sizes and better integration with photonic devices than the commonly available fiber amplifiers. However, on-chip amplifiers have yet to make its way into the mainstream due to the limited availability of materials with ideal light guiding and amplification properties. Polymeric waveguide amplifiers (PWA) comprising of Er-doped nanocrystals dispersed within polymers offer an attractive low-cost solution towards creating high gain on chip amplifiers that have a small device footprint and also integrates well with devices. In this work, we have synthesized an active PWA core comprising of surface-modified tri-doped NaYF₄ nanoparticles (N-NPs) that are dispersed within a SU8 polymer. The nanoparticle design and synthesis that led to enhanced IR emission efficiency by controlling its dopant chemistry will be discussed. We will also present about the fabrication of efficient IR-emitting composites that exhibit mostly single particle dispersion at high loading by tailoring the interfacial chemistries using an amphiphilic surfactant. The typical range of the polymer refractive indices poses an interesting material and device design conundrum. Although the range of refractive indices for most polymers is advantageous towards designing the low-loss active composite core, it is actually detrimental from the waveguide device design perspective. The small index mismatch between the nanoparticle and polymer ($dn = 0.03-0.06$) leads to reduced losses at the particle-polymer interface. However, this also leads to an undesired low index contrast ($dn = 0.03-0.12$) at the active core-SiO₂ cladding interface for conventional waveguide design resulting in poor light confinement. In this talk, we present a unique air-cladded channel waveguide structure design which increases the core-cladding interface index contrast to ~ 0.58 to maximize light confinement. Using our composites and waveguide design, we measured one of the highest gain to date of 6.6 dB/cm at a coupled pump power of 80 mW. The high gain is attributed to: (1) bright IR emissions from our nanoparticles, (2) uniform particle dispersion at high loading using our surface modification strategy and (3) improved mode confinement using our air-cladded channel design.

Abstract ID: 570

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Lithium Ion Batteries

Keywords: Double-wall carbon nanotubes, Shuttle effect, Modified separator, Lithium sulfur batteries, Energy storage materials

Double-Walled Carbon Nanotubes Used for Enhanced Lithium-Sulfur Batteries

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Lithium-sulfur (Li-S) batteries are considered as next generation batteries for energy storage systems due to its high energy density. However, the rapid capacity fading resulted from the shuttle effect obstructs its practical applications. Herein, double-walled carbon nanotubes (DWCNT)-modified separator has been designed to impede the shuttle effect. For the DWCNT, its outer wall helps to keep the integrity and conductivity of its inner wall. And also, the defects of oxidized DWCNT, less than normal used multi-walled CNT (MWCNT), contributes to the better conductivity. Compared to MWCNTs, the DWCNTs was found in our work to be helpful for the Li-S battery's performance. Especially, the cycling stability of Li-S batteries have been effectively improved with the DWCNTs applied. This work offers a possible solution to solve the shuttle effect of polysulfides for Li-S batteries.

Abstract ID: 571

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Chemistry of 2D Materials for Energy, Catalysis and Sensing Applications

Keywords: Renewable Copper Nano-Clusters, Electrochemical Sensor, Nitrate Determination

An Electrochemical Sensor Modified with Renewable Copper Nano-Clusters for Continuous Nitrate Determination

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Recently growing concern has been expressed on nitrate ions for its potential threat towards aquatic ecosystems and human health. Lots of studies have proved that excessive nitrate ions enriched in aquatic systems can present both environmental and physiological problems. So it is clear that monitoring nitrate concentration in aqueous samples is very important. Copper nanomaterials have been demonstrated to be an effective electrocatalyst for direct electroanalytical determination of nitrate ions in solutions. Lots of electrochemical sensors modified by copper nanomaterials have been reported to have sufficient sensitivity for nitrate detection in natural waters. However, due to the surface cumulative passivation effects, the decreasing sensitivity towards analytical target has restricted the long term applications of these devices. In this paper, an electrochemical sensor based on renewable copper nano-clusters modified microelectrode for nitrate measurement is presented. A micro three-electrode-system was fabricated to implement sensitive, reproducible and continuous nitrate measurements under a programmed operation protocol. Based on the optimized potential protocol, the continuous renewal of copper sensing material was achieved on the working-electrode surface to ensure each measurement could be performed on a fresh and highly active copper surface, which guaranteed that continuous nitrate determination could be performed in a long period of time. The experiment results revealed that the response of the sensor toward standard nitrate samples was linear and reproducible with an average sensitivity of $1.093 \mu\text{A}/\text{mgL}^{-1}$ over the concentration range from 0 to 12.1 mg/L in a continuous long-term operation. The standard deviation for the fluctuation of the sensitivity is only 0.036 during the continuous repeated measurements. The difference of 20 times measurements for one sample was determined as 4.8% at the optimized conditions, which shows good repeatability of the sensor. This study offers a promising route to greatly enhance the practicability of electrochemical sensors in environmental sample analysis.

Abstract ID: 572

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Transport and systems modeling

Keywords: Millimeterwave, Sintering, Phase

Physics of the dielectric properties of microwave and millimeterwave ceramics

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at the start of the 20th century, electromagnetic signals were sent by Marconi across the Atlantic Ocean which led to the invention of radio communications [1]. After that wireless mobile systems were realized during 1940. The growth in the wireless mobile markets is witnessed at the start of the 21 century fueled by an information explosion. This became possible by the utilization of dielectric materials as resonator, filter and oscillator due to the unique dielectric properties namely permittivity, quality factor and temperature coefficient of resonant frequency. Dielectric Resonator is the key component in any microwave telecommunication devices. The value of permittivity decides about the use of ceramics for a particular application. For high performance devices application, a high quality factor is needed because the higher the quality factor, the higher will be the efficiency and lower is the noise. The resonant frequency must be stable to variation in the temperature of its operating environment for practical application of a resonator. Research and development in telecommunication enabled the investigation in the utilization of different ceramics with different range of the dielectric properties. There are three categories encompassing research and development of microwave and millimeterwave dielectric materials in the ever-present age. The first category of dielectrics with high relative permittivity ($\epsilon_r > 80$) and $Q_{\text{fwhm}} < 10,000$ GHz find application in mobile phones where reduction of the device size is very important. The second category of dielectrics with medium relative permittivity ($20 < \epsilon_r < 30,000$) are used in filters for satellite communication and cellular phone base stations. The third category of dielectric materials with low permittivity ($\epsilon_r < 15$) and ultra-high $Q_{\text{fwhm}} > 70,000$ GHz are used for millimeterwave and substrate applications. These properties are greatly affected by numerous factors that includes compositional variation, order/disorder behavior, Dark core formation, compositional ordering, microstructure, grain size, grain boundaries, humidity, porosity, octahedral tilting transition. Tolerance factor, Control over these factors could be possible by utilizing the knowledge and concepts of Physics.

Abstract ID: 573

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Invited Talk

Topics: Diagnostic and therapeutic biomaterials

Keywords: Programmable materials, Biomaterials, Nanomaterials, Theranostics

Advanced Functional Biomaterials for Programmable Theranostics

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Theranostics is the advanced solicitations of exploiting intelligent material properties to clinical medicine for simultaneous diagnosis and therapy. The perception of personalized medicine will depend on the success of theranostics where drug will be anchored as “companion” with the in-built diagnostic system to precisely govern whether the patient will get benefit from the particular treatment, and to real time monitor the therapeutic progression to determine the curative efficacy. The concept involves molecular level on site diagnosis and directed therapy in an inter-reliant, co-operative patient profile-based way for individualized treatment. This arrangement of drug module to target a disease condition on an individual basis as a straightforward consequence of the intelligence derivative from on spot diagnosis is the most ambient strategy require today to combat complex heterogeneous disease such as cancer. We have developed and examine how programmable materials are becoming important part for the biomedical systems and providing new insights into targeted therapy and spurring significant advancement in the fields of regenerative medicine, tissue engineering and heterogeneous complex disease like inflammation, cancer etc. This presentation will therefore highlight the current advances in the development on the programming of such theranostic systems and how such advanced ideas could be translated into on/off switchable medicine to meet the fundamental goal of personalized medicine.

Abstract ID: 574

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Fiber reinforced Composites

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

Cement-based composites with Short Carbon Fibers for Self Sensing Properties

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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: 575

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Composites in Innovative Applications

Keywords: rotary swaging; laminated composite; clad composite; electric conductivity; residual stress

Innovative Cu/Al laminated composite wire conductors: effect of rotary swaging on electric properties and structural characteristics

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Laminated and clad composites are modern materials, consisting of at least two different materials bond at adjoining interfaces, gaining increasing interest in various industrial and commercial branches. This study is focused on the investigation of innovative, uniquely sequenced Cu-Al laminated composite wires perspective for various applications, from transportation to electrotechnics. The composites were manufactured via the versatile technology of rotary swaging enabling manufacture of various axially symmetrical products via repeated action of the rotating dies. Rotary swaging was performed at 20 °C and 250 °C down to the composite diameter of 5 mm, with the swaging degree to 3.6. The subsequent analyses focused on the influence of the swaging degree and temperature on the mechanical and electric properties, as well as the development of substructure and residual stress. After swaging, both the Al and Cu 5 mm composite wires components exhibited recrystallized ultra-fine-grained structures with decreased levels of residual stress. The electric resistivity was generally higher for the wires swaged at 250 °C, primarily due to the occurrence of intermetallics, and for the pre-final swaging passes, the material during which exhibited deformation hardening; it was the lowest for the restored structures of 7.5 mm and 5 mm composite wires ($0.0165 \Omega \cdot \text{mm}^2 \cdot \text{m}^{-1}$).

Wednesday, 21/Aug/2019 4:12pm - 4:24pm

Abstract ID: 576 / FBB-2: 2

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biomaterials for Cardiovascular Applications

Keywords: cardiomyocyte, contraction force, piezoelectric cantilever sensor

Direct measurement of human derived cardiomyocyte cluster contraction force using piezoelectric cantilever sensor

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Human stem cell based tissue and organ models to study toxicology and diseases are ethically beneficial and more trustworthy over the animal experimentation. Development of real-time cardiovascular model for personal medicine and drug development using patient's own stem cells requires highly developed cell biology combined with highly sensitive measurement technology and in-situ microscopy techniques. During recent years, various techniques for cardiomyocyte contraction force measurements has been reported [1-5]. In this paper, we demonstrate a proof-of-concept technique for direct contraction force measurements for human cardiomyocyte clusters under microscope. The culturing of cardiomyocyte clusters was performed by technique adapted from the previous work [6-7]. Highly sensitive force sensors were contracted from a metallic cantilever attached to a piezoelectric sensor, which was connected to in-house build dedicated hardware and user interface plate. The measurement system was further developed version from a previously work [8].

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Abstract ID: 578

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Porous and cellular materials

Keywords: Superoleophilic, Oil-water separation, Ultra-high flux, Electrophoretic deposition

Ultra-high flux and efficient oil-water separation via polymer-based electrophoretic deposition

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An environmentally-friendly hydrophobic and superoleophilic membrane was successfully fabricated on a stainless steel mesh via a facile electrophoretic deposition process. The contact angles of water and n-hexane on the modified mesh were $125 \pm 5^\circ$ and $< 10^\circ$, respectively. Oil passed through the membrane within only 15 s despite being solely driven by gravity, showing an ultra-high flux (above $15000 \text{ L}\cdot\text{m}^{-2}\cdot\text{h}^{-1}$) and a very high oil-water separation efficiency (above 99.5%). The separation efficiency of the prepared membrane remained above 99.0% after treatment in various harsh environments, including acid (pH 0), alkaline (pH 14) media as well as concentrated brine for 24 h. This study provides a cost-efficient method to prepare stable water-soluble silicon-containing polyacrylate (WSPA) membranes on stainless steel meshes without using toxic fluorinated compounds, which has significantly promising practical applications for oil-water separation.

Abstract ID: 579

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

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

Keywords: Energy harvesting, stochastic resonance, Mean residence time, stability

Stochastic resonance and time-delayed feedback control of nonlinear electromechanical energy harvester under random excitation

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Energy harvesting, known also as energy scavenging, covers a great body of technologies and devices that transform low grade energy sources such as solar energy, environmental vibrations, thermal energy, and human motion into usable electrical energy. Thanks to the recent technology progress recorded in the electronic domain, the electrical energy consumption by the electronics components has dramatically decreased, incited the proliferation of the wireless devices. Thus, the energy harvesting technology has become a very attractive solution for a wide variety of applications such as consumer electronics, outpatient medical electronics (hearing aids, pacemakers, smart implants) or imaging (camera inside the human body). In this manuscript, a hybrid energy scavenging system combining piezoelectric and electromagnetic transduction and subjected to the random noise is investigated. By using the stochastic averaging method, the statistic response of the system is assessed and reveals interesting dynamics related to the long term behavior of the device. From this statistic response, we analyze the harvester stability. Numerical simulations are made for a comparison with analytical findings. By computing the Mean residence time (TMR), we explore the stochastic resonance phenomenon; we show how it is related to the noise parameters and high output power.

Abstract ID: 580

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Photocatalytic and electrochemical water splitting

Keywords: Photocatalysis, Gallium Niobate, Water splitting

Optical properties of site specific S and Se doping in GaNbO₄

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GaNbO₄, a wide bandgap semiconductor has an indirect bandgap of 3.2 eV which is close to that of TiO₂ the most widely studied photocatalyst. Earlier experiments on GaNbO₄ investigating its photocatalytic activity found that it can dissociate water under UV light [1] and that doping with sulphur shows promise of photocatalytic activity in the visible range. We have performed electronic structure calculations on pure and doped GaNbO₄ to understand the effect of dopant on the band gap reduction and as a consequence on the optical properties. Our investigations show that S and Se doping reduces the bandgap. The reduction in band gap has a dependence on the dopant site. The optical properties are seen to be site dependent. S and Se doping of GaNbO₄ induces absorption in the visible range along with enhancement and broadening of the absorbance peaks in the UV region. Increasing the dopant concentration leads to a further reduction in the band gaps and enhancement of the absorbance peak in the visible region. We discuss the differences in the absorption of doped and undoped GaNbO₄ with that of the rutile and anatase phase of TiO₂.

Abstract ID: 581

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Nanomaterials for Biomedical Applications

Keywords: Denture Liners, nanotechnology, mechanical properties.

Self-curing reline resin with antimicrobial activity

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Polymeric liners for dental use, based on poly-methyl methacrylate or silicone, are used for rebuilding the surface of the prosthesis in contact with the oral mucosa. They are widely used in clinical practice, however, its major disadvantage is the easy microbial contamination as a function of the porosities derived from its structural formation, composition, and properties. Liner contamination may cause serious local problems such as implant loss in addition to systemic diseases such as bacterial endocarditis and pneumonia. We incorporate nanostructured silver vanadate decorated with silver nanoparticles (AgVO₃) at different concentrations to a resin denture liner and evaluate the antimicrobial capacity, adhesion properties, hardness, and roughness. AgVO₃ added to the reline resin at concentrations of 1 and 2.5% showed antimicrobial activity for *E. faecalis*, and 5 and 10% were effective for *E. faecalis*, *P. aeruginosa* and *C. albicans*. There was a decrease in hardness for the 1, 2.5, and 10% AgVO₃ concentrations while in the 5% group, this property remained unchanged ($p < 0.001$). None of tested concentrations significantly changed the roughness of the material but a significant increase in tensile bond strength was found in the 2.5% ($p < 0.001$) and 10% groups ($p = 0.042$). This study showed that 5% AgVO₃ incorporation to a soft denture liner promoted antimicrobial activity without affecting roughness, AgVO₃ at 1% maintained the hardness properties recommended for soft and extra soft liners, and AgVO₃ at 2.5% improved the adhesion between the liner and the acrylic resin used for dentures.

Abstract ID: 582

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

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

Keywords: contact force, friction layer model, electromechanical conversion efficiency, circular cylindrical wedge wave ultrasonic motor

Contact force analysis of a circular cylindrical wedge wave ultrasonic motor

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A circular cylindrical wedge wave ultrasonic motor is a novel actuator that generates traveling waves under high-frequency vibration created by its stator and uses contact force to actuate the rotor's rotation. The most important issues include the stator-rotor friction layer model and material parameters. Thus, this study used contact mechanics analysis to explore various available friction layer models and material parameters to improve the efficiency and step integrity of a wedge wave ultrasonic motor. The driving method of the completed prototype of a circular cylindrical wedge wave ultrasonic motor was applied. The commercial software 3D ANSYS was used to analyze the stator-rotor friction layer model and simulate the mechanism of transient responses between the stator and rotor. Under given external force and displacement boundary conditions, ideal convergence parameters and reasonable calculation results were selected to determine the optimal friction layer parameters. Performance curves were used to estimate the rotational speed and torque of a circular cylindrical wedge wave ultrasonic motor. In this study, a stator-rotor friction layer model was established and an equation expressing relations between contact stress and strain in wedge waves was developed, as shown in Figure 1. The 3D ANSYS simulation results demonstrated that the application of an accurate stator-rotor friction layer model and appropriate material parameters can improve the electromechanical conversion efficiency of a circular cylindrical wedge wave ultrasonic motor.

Abstract ID: 583

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Lab-on-a-chip

Keywords: microfluidics, ultrasounds, lab-on-a-chip, cell micromanipulation, cell sorting, aggregation

Low-cost microfluidic devices to perform cell manipulation by ultrasounds

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Polymeric microfluidic devices implemented by ultrasonic actuators provide a promising high-throughput technology to perform particle or cell manipulation with diverse applications in the framework of biomedical and environmental disciplines. These devices integrate acoustic and hydrodynamic mechanisms in their performance to generate different cell aggregation or sorting desired effects, depending on the specific application.

The presence of circulating tumor cells (CTCs) in peripheral blood have become established as biomarkers of prognosis and may be useful as an early indicator of tumor spread, as invasive but localized tumors may shed CTCs into the bloodstream before the establishment of a metastasis. Detecting, isolating, and analyzing CTCs has the potential to improve diagnosis, allow prognostic monitoring, and enable targeted treatment strategies that are based on the metastatic cells mainly responsible for cancer mortality. However, they are challenging to isolate.

We developed polymer-based chips with different geometry and actuation based on the actuation of ultrasounds strategically applied to perform versatile cell collection along their channelization, susceptible of positional variations during the acoustic treatment. We introduced the concept of plate-vibrations in the development of a new polymeric acoustophoretic chip actuated by a single piezoelectric transducer to perform high-throughput isolation of tumor cells from flowing blood samples, and BULK wave-based polymeric chips with lower frequencial stability but highly reversible in frequency. Both types of chips have provided highly efficient results. This low-cost technology offers a promising route forward clinical applications, even allowing printing manufacturing, unlike conventional Bulk-based microseparators.

Abstract ID: 584

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Environmental Catalysis

Keywords: Iron-doped TiO₂, Photo-catalysis, hydroxyl radical, mechanism

Efficiency and Mechanisms of Mesoporous Iron-Titanium oxides to generate hydroxyl radicals for degradation of Acid Orange 7 Dye

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As small amount of iron (0.2 weight %) doped on titanium oxides (Fe/TiO₂) surface, the mineralization of Acid Orange 7 (AO7) dye was increased more than 50% under visual light photo-catalysis than that of P25-TiO₂ owing to the reduction of Band-gap between Valance Band (VB) and Conduction Band (CB). It was found that the generation of hydroxyl radicals (HRs) was more than double through mainly from the VB position of Fe/TiO₂ by the observation through controlling the dissolved oxygen. The contributions of HRs from VB under ultra-violet (UV) and visual light (VL) were about the same at 56 and 58%--slightly more than those by CB. The mineralization started to break N=N double bonds by HRs or additive hydroxyl to naphthalene ring on AO7 at low Reaction Efficiency (RE) during photo-catalysis and to break naphthalene rings at high RE through the analysis of Liquid Chromatography Mass Spectrum (LCMS). It was inferred that the doped iron could reduce the re-combination of free electron among CB and VB and enhance HRs generation mechanisms under photo-catalysis by UV and VL.

Wednesday, 21/Aug/2019 5:12pm - 5:24pm

Abstract ID: 585 / FBB: 7

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Application of Biosensors in Drug Delivery and Clinical Chemistry

Keywords: Environmental protection, Forensic Medicine, Biosensor, Contaminants, Nanotechnology.

The Applications of Nanotechnology Based Biosensors

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Biosensors is an analytical instrument, it is mostly used to detect a biological component like biological catalyst (Enzyme), DNA, Animal Cell. In developing biosensors, Nanotechnology is playing a vital role. Biosensors are designed to carryout a range of functions like routine analysis, such as water quality control, security of Nations. It is also applied in clinical diagnosis and Forensic medicine. In environmental protection and management these are used in the detection of contaminants like heavy metal ions, like lead, and genome analysis of organisms and their communications within an area. The construction of biosensors using Nanomaterials has improved its efficiency. The development of different tool and the processes used in fabrications measure and image nanoscale objects has led to designing of sensors that interact with highly small molecules. There are several Nanobiosensor based optical resonators, nanowires, nanotubes and nanoparticles, carbon nanotubes and others have been investigated and confirmed for their application in biosensors, which have become a new link between biological detection and other field of sciences like material sciences. With the development of Nanotechnology and its vital role in developing ultrasensitive instruments, it can be said that it is one of the most promising way to solve a range of problem concerning the increasing need to develop a highly sensitive, quick and economic method to carry out analysis in Medicine and Environmental protection and management

Keyword: Environmental protection, Forensic Medicine, Biosensor, Contaminants, Nanotechnology.

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Abstract ID: 586

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Advances in Enzymatic and Non-Enzymatic Biosensors

Keywords: 3, 3', 5, 5 tetramethylbenzidine (TMB), blood glucose, Glucose Oxidase (GOx), Hydrogen Peroxide (H₂O₂), Colorimetric detection, Core-shell structured Fe₃O₄@C

Fe₃O₄@C core-shell structure: Peroxidase -Like Activity for Development of A Colorimetric Sensor For Glucose Detection. Application to Human Serum

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In this study, we present a simple synthesis method for preparation of Fe₃O₄@C core-shell structure nanocomposite by hydrothermal method. Fe₃O₄@C nanocomposite was characterized by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM)/Transmission Electron Microscopy (TEM), Fourier-Transform Infrared spectroscopy (FT-IR) and Vibrating Sample Magnetometer (VSM) methods. Obtained results showed that Fe₃O₄@C nanocomposite with core-shell structure, the core is Fe₃O₄ particles with diameter of 11-14 nm and amorphous carbon as shell layer with thickness was 1.2 - 1.5 nm. The synthesized Fe₃O₄/C nanocomposite has performed excellent catalytic activity similar to peroxidase for catalyzing the reaction between 3,3',5,5 tetramethylbenzidine(TMB) with hydrogen peroxide (H₂O₂) to produce TMB from colorless (reduced state) to oxidation state as blue color. The Fe₃O₄@C nanocomposite has a high catalytic activity therefore; an ultrasensitive colorimetric sensor for hydrogen peroxide detection was described with low detection limits of 100 nM of H₂O₂. Basing hydrogen peroxide sensor, we also employed glucose oxidase enzyme (GOx) to fabricate a colorimetric bio-sensor for glucose detection. Proposed glucose sensor performed excellent selectivity to glucose and very high sensitivity with LOD of 300 nM glucose.

Wednesday, 21/Aug/2019 4:36pm - 4:48pm

Abstract ID: 587 / FCM: 4

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Smart Composites

Keywords: Ionogel, smart material, responsive material, wetting

Responsive Ionogel with Switchable Surface Properties

Werner Steffen, Ye Lijun, Chen Fei, Jie Liu, Aiting Gao, Gunnar Kircher, Julian Mars, Kamal Asadi, Markus Mezger, Michael Kappl, Seraphine Wegner, Hans-Jürgen Butt

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By mixing a polymer and an ionic liquid a temperature responsive material with a switching temperature in the range from 37°C to 55°C was synthesized. Our ionogel spontaneously forms an interdigitated two-phase material on cooling from high temperatures or under controlled evaporation of a common solvent. Depending on temperature, the ionic liquid is crystalline or liquid. The crystallites and the highly viscous amorphous part of the polymer serve as a robust framework below the T_m (120°C) of the polymer providing mechanical stability. The solid-liquid transitions of the ionic liquid causes a transformation of the ionogel into a solid and back to the liquid state, leading to significant – reversible - changes in elasticity, ion conductivity, transparency and wettability. We set the temperature range of switching via combinations of different side groups of the ionic liquid. The reversibility of the “solid-gel” transition together with the negligible vapor pressure and excellent thermal stability of ionic liquids provide a durable switch of these physicochemical properties of this new type of ionogel material.

Abstract ID: 588

Symposium 5: Functional 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, CNT, TMD, hybrid film, photodetection

Growth of CNT-weaved 2D hybrid films for flexible electronics

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Two-dimensional materials have attracted much attention due to their unique structure and excellent electrical and mechanical properties. With the CNT spider-web network as the template, we synthesized series of robust and CNT-weaved graphene/CNT and transition metal dichalcogenide(TMD)/CNT hybrid films. A unique growth mechanism of the 2D films with the existence of CNTs was observed and proposed. We further developed a general method to chemically grow large-area and seamless transistors with the hybrid films as the electrodes and graphene and TMD as the channels. These seamless devices exhibit excellent mechanical stability and high sensitivity in in vivo electrophysiological mapping of rat cardiac signals and photodetection. Graphene/CNT hybrid films based wearable electronics with high sensitivity and large linearity range were also developed.

Key Words: Graphene, CNT, TMD, hybrid film, photodetection

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Abstract ID: 589

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Structural, electrical, mechanical and optical of low dimensional, nano and 2D-layered oxides, nitrides and sulfides

Keywords: Bi(Na, Ti)O₃, Lead-free, Piezoelectric, Dielectric, Colloidal Coating

Synthesis of (Bi,Na)TiO₃ nanoparticles by Colloidal Coating Method and Their Dielectric and Piezoelectric Properties

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Piezoelectric ceramics which can convert mechanical energy to electrical energy and vice versa, are used in electromechanical applications such as sensors, actuators, and transducers. These application areas are utilized in automotive, military, medical, and etc. Mostly lead-based ceramics (e.g. lead zirconium titanate, PZT and lead magnesium niobate-lead titanate, PMN-PT) are preferred for such applications due to their high piezoelectric performance. The regulatory sanctions of the European Union on the elimination of toxic materials in electrical and electronic equipment led to an intense research activity in the reduction and removal of lead, which is harmful to environment and health, in the aforementioned applications.

Various lead-free ceramic systems like potassium sodium niobate (KNN), bismuth sodium titanate (BNT), bismuth iron oxide (BF), sodium tantalate (NT), and barium calcium titanium zirconate (BCTZ) have been considered as potential candidates instead of their lead-based counterparts. Among these materials, BNT-based ceramics come into prominence due to their high piezoelectric constant value. Solid solution between BNT and bismuth potassium titanate (BKT) is a promising alternative to lead-based systems since it exhibits a high strain value and a similar phase diagram to that of PZT binary system (lead titanate, PT – lead zirconate, PZ).

However, volatility of Bi, Na, and K during high temperature sintering using conventional mixed-oxide method causes deterioration of the initial stoichiometry of BNT and BNT-BKT based compositions. In addition, non-stoichiometric compositions lead to formation of secondary and undesired phases (K₄Ti₃O₈, K₂Ti₆O₁₃, NaBiTi₆O₁₄) during production which in turn worsen the electrical properties. Colloidal coating method is a solution based ceramic powder synthesis technique. It was used in the successful elimination of pyrochlore phase formation in the lead-based compositions such as PMN-PT. This method also makes the production of nanometer-sized particles possible. Since the atomic diffusion kinetics between these particles during sintering is very high, it enables the production of high-density ceramics at lower sintering temperatures. The main aim of this study is the employment of colloidal coating technique in the production of ceramic powders of BNT-based systems. Preliminary experimental results revealed that a more homogeneous mixing of the starting powders and purer BNT powder can be obtained by the solution coating approach compared to the conventional mixed-oxide method.

Abstract ID: 590

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Composite structural materials

Keywords: direct carbonization, chemical vapour deposition, microstructure, mechanical strength, thermal conductivity

Three-dimensional reticulation SiC/porous carbon foam aerogel composites for thermal insulation devices

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Generally, glass fiber reinforced silica aerogels showed high intensity and low density. In this paper, the SiC/porous carbon foam (PCF) network was acted as the reinforcing skeleton, and silica aerogel was inducted into the pore structure via atmospheric pressure drying method. The microstructure, mechanical strength, and thermal properties of the as-prepared SiC/PCF aerogel composite were studied. The results showed that a novel three-dimensional SiC skeleton having an open-cell network with silica aerogel was fabricated successfully. The thickness of the SiC coating had a significant influence on the compression and thermal properties of the composites. Besides, the thermal conductivity of the final composite was much lower than that of PCF and SiC/PCF. This present work had some reference meaning to the correlation studies of the thermal insulation material for the potential applications while bearing live loads.

Abstract ID:591 / Poster: 38

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Biomaterials for musculoskeletal regenerative engineering

Keywords: Self-organization of cells, Biomaterials, Hydrogels, Myoblasts

Self-organizing Behaviors of Murine Myoblasts in the Dextran Hydrogel with Adjustable Configuration

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Biomaterials serves important functions for regenerating tissues or restore tissue function has become impaired by chronic degeneration or physical damages. The cell-compatible biomaterials need to provide a suitable extracellular matrix for the encapsulated cells and cytokines to induce cells to self-organize into the predicted tissue structures. However, the self-organization mechanism underlying the multicellular structure formation inside 3D biomaterials is still unclear. Here, a specific designed dextran-based hydrogel was used as the 3D matrix whose components including polymer, cross-linker and adhesion peptide can be quantitatively configured. The murine myoblast cell line C2C12 was cultured for one week in this dextran-based hydrogel. The viability, spread and migration of the C2C12 cells in 3D Dextran-based hydrogel were examined by bright field, immunofluorescent and confocal microscopy. The micrographs were quantitatively analyzed. The results show that the cells sprouted and spread earlier with a large extent of elongation with lower cross-linking strength (the concentration of cross-linkers < 2.5 mM); while the cells kept round-shape or small extent of sprouting and spreading with larger cross-linking strength (> 3.5 mM). The C2C12 cells did not obviously spread quicker or with larger extent of spreading when the concentration of RGD peptides is larger than $400 \mu\text{M}$. At the optimized conditions with 2.0 mM crosslinkers and $300 \mu\text{M}$ RGD peptides, quite a few C2C12 cells had stretched themselves into a much more slender strip, then they aggregated in parallelly aligned style and the self-organized slender aggregates of cells become thicker and longer over time. Some individual cells could even stretch dozens of times their original length in this hydrogel. Our study produces a robust 3D culture model with a hydrogel whose ingredient proportion can be quantitatively tailored, which lays a solid foundation for tissue regenerating or drug testing with adjustable configuration of hydrogel.

Abstract ID: 592

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Biomimetic materials

Keywords: Perovskite, Imprinting, Photoelectrochemical, Sensor

Molecular imprinted organometal lead halide perovskites: an effective platform for constructing sensitive and selective photoelectrochemical sensor

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The hybrid organic-inorganic lead halide perovskite materials have attracted much attention in recent years due to their excellent optical and electrical properties. This work integrated the good photoelectrochemical character of lead halide perovskite and the excellent selectivity of molecular imprinted polymers together to establish a novel photoelectrochemical sensor for the detection of salicylic acid. Fig. 1 illustrated the photoelectrochemical sensor construction process. This work extended the application of perovskite materials into a new area. Scanning electron microscopys confirmed the imprinting of salicylic acid on lead halide perovskite. Under the optimal conditions, the photoelectrochemical sensor showed a linearity from 7.0×10^{-13} to 1.0×10^{-8} M to salicylic acid. The detection limit was down to 1.95×10^{-13} M. The established photoelectrochemical sensor has been used successfully to detect salicylic acid directly in medicine samples.

Abstract ID: 593

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Superconducting and magnetic materials

Keywords: Single domain GdBCO bulk and ring, Gd+011 TSIG method, trapped field, theoretical and numerical calculation

Theoretical and numerical calculation of trapped field distribution of single domain GdBCO bulk and ring superconductors by Gd+011 TSIG methods

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In this paper, a single domain GdBCO bulk sample S1 ($\phi 32\text{mm}$) and a single domain ring samples S2 ($\phi 32\text{ mm}$, with an inner hole of 10 mm in diameter) have been fabricated in air by a new Gd+011 TSIG method. The trapped field of the samples is 0.32 T and 0.33 T at liquid nitrogen temperature for the samples S1 and S2 respectively, The trapped field mapping were carried out by a Hall probe after samples were magnetized at 0.50 T under field-cooled (FC) state. The trapped field uniformity of ring is much better than that of the single domain GdBCO bulk superconductors. The details have been explained by theoretical and numerical simulation of single domain GdBCO bulk and rings based on the electromagnetic knowledge.

Wednesday, 21/Aug/2019 5:27pm - 5:39pm

Abstract ID: 594 / FC: 8

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Nano and Environmental catalysis

Keywords: Sub 1 nm Cu nps, high intensity ultrasound sonication, 1, 2, 3-triazole.

Synthesis and characterization of sub 1 nm poly(acrylic acid) capped copper nanoparticles using high intensity (30 KHz) ultrasound sonication and their catalytic study

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Synthesis and characterization of sub 1 nm poly(acrylic acid) capped copper nanoparticles using high intensity (30 KHz) ultrasound sonication and their catalytic study

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The sub 1 nm size poly(acrylic acid) capped copper nanoparticles were synthesized by using high intensity (30 KHz) ultrasound sonication method. The reduction of copper NPs from copper(II) salt by L-ascorbic acid in water medium was achieved in the presence of poly(acrylic acid) by high intensity (30 KHz) ultrasound sonication. The poly(acrylic acid) capped copper nanoparticles (PAACC NPs) were characterized by DRS UV-Visible, XPS, FESEM and HRTEM techniques. The Huisgen 1,3-dipolar cycloaddition reaction between azides and terminal alkynes is possibly the most well-known “click ” reaction and has made a durable inscription on synthetic, biological and industrial chemistry. The PAACC NPs exhibit high catalytic activity towards the synthesis of 1,2,3-triazole compounds via click reaction under mild reaction condition, excellent regioselectivity and are eco-friendly . Recently, benzoxazole and benzothiazole capped triazole compounds have been applied as additives in DSSCs and organic light emitting materials.

Keywords: Sub 1 nm Cu nps, high intensity ultrasound sonication, 1,2,3-triazole.

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- FESEM image(A)EDAX pattern(B), HRTEM image(C) and (D) SAED pattern of PAACC NPs

Abstract ID: 595

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Superconducting and magnetic materials

Keywords: Single domain GdBCO bulk and ring, Gd+011 TSIG method, trapped field, theoretical and numerical calculation

Theoretical and numerical calculation of trapped field distribution of single domain GdBCO bulk and ring superconductors by Gd+011 TSIG methods

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In this paper, a single domain GdBCO bulk sample S1 ($\phi 32\text{mm}$) and a single domain ring samples S2 ($\phi 32\text{ mm}$, with an inner hole of 10 mm in diameter) have been fabricated in air by a new Gd+011 TSIG method. The trapped field of the samples is 0.32 T and 0.33 T at liquid nitrogen temperature for the samples S1 and S2 respectively, The trapped field mapping were carried out by a Hall probe after samples were magnetized at 0.50 T under field-cooled (FC) state. The trapped field uniformity of ring is much better than that of the single domain GdBCO bulk superconductors. The details have been explained by theoretical and numerical simulation of single domain GdBCO bulk and rings based on the electromagnetic knowledge.

Thursday, 22/Aug/2019 11:48am - 12:00pm

Abstract ID: 596 / FTF: 5

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: EUV-Soft-X-ray multilayers

Keywords: XUV/x-ray Laser, Surface Modification, Multilayer, Fullerene

Radiation processing of functional materials with XUV/x-ray laser pulses

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The first soft x-ray laser was put into operation in Livermore (CA, USA) more than three decades ago [1]. The development of both plasma- and e-beam-based short-wavelength lasers and measurements of their output characteristics are briefly reviewed in the talk. Special attention is paid to extreme ultraviolet (XUV) and soft x-ray free-electron lasers (FEL) and their prospective transformation from large-scale facilities to compact sources available in standard laboratories. Some specific advantages and drawbacks of certain XUV/x-ray lasers are treated with respect to their applications in direct radiation processing of functional materials. Ablation, desorption and solid-to-solid phase-transition processes [2] induced by high fluxes of energetic photons are introduced in the talk. The difference in an action of short and ultra-short pulses of XUV/x-ray laser radiation is pointed out. A key advantage of these lasers for fabrication of tailored nanostructures lies in the unique combination of exceptionally short wavelength, high degree of coherence, and enormous peak power. Certain thresholds for materials processing require XUV/x-ray sources to deliver enough radiation power to the irradiated surface area. Although high-order harmonics and incoherent sources developed for XUV/x-ray lithography can also pattern material surfaces with nanometer precision, they cannot directly produce three-dimensional nanostructures using a few shots in a single processing step. It has been demonstrated that intense XUV/x-ray laser radiation can produce submicron structures directly. Grating-like structures (i.e., LIPSS - laser-induced periodic surface structures) with a spatial period of ~ 70 nm have already been spontaneously formed on amorphous carbon - a-C [3] and poly(methyl methacrylate) - PMMA [4] surfaces irradiated with 98-nm and 86-nm FEL radiation, respectively. However, an abundance of these patterns on FEL-irradiated surfaces is very low. There is one promising exception. Surprisingly high abundance of LIPSS with a spatial period of 65 nm was registered on Si/Mo multilayer irradiated by a FEL source tuned at 13.7 nm. Mechanism of their formation is not yet clarified. Some recent results obtained on carbonaceous materials are described in details. For example, the phenomenon of the intermolecular Coulomb explosion has been registered in fullerene thin films exposed to short-wavelength FEL radiation [5].

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Abstract ID: 597

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Solar Cells

Keywords: Perovskite solar cell, Water soluble, Lead precursor

Investigation of nanostructured thin films based on water soluble precursors for perovskite solar cells

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The objective of this study has been to develop water soluble processes for high efficiency perovskite solar cells. Fluorine-tin oxide-coated glass substrate was cleaned, then surface-treated with plasma and UV light irradiation to increase its hydrophilicity. The electron-transport layer, composed of titanium dioxide dense layer and a mesoporous layer, was spin-coated and further annealed. A precursor solution of lead nitrate was used to deposit lead dioxide film, which was then immersed in MAI to create the MAPbI₃ perovskite nanostructured thin film. Spiro-OMeTAD was used as the hole-transport layer, and silver was applied as the cathode. The contact angle analysis suggested that 20 min under the UV-ozone treatment was enough to provide a good surface condition for coating. In addition, the solar cell C-V performances under the various lead nitrate precursor concentrations have been studied. The conversion efficiency was achieved at higher than 10.0%. Since the development of less toxic, water-based precursor formulation, it has been encouraging to find better deposition method for lead precursor, thus the perovskite nanostructure. After the parameters have been optimized, long time stability characterization could be carried out for the new high efficient perovskite solar cells. The new results will be presented and discussed in greater details.

Abstract ID: 598

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Polymeric composites

Keywords: Graphene oxide, phenolic resin, dielectric, tunable

Graphene oxide/ phenolic resin nanocomposite fibers with high-strength, towards and dielectric tunable performance

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Requirements for the variable and multifunctional fiber has substantially increased in textile industry, information detection, aerospace, and biotechnological applications. This research explores to synthesize nanocomposite functional fibers by modifying phenolic resin (PR) with graphene oxide (GO) and controlling assignment orientation of GO in the PR matrix. The GO/PR nanocomposite fibers were prepared via gel spinning and subsequent hot drawing process. Results shown that GO was reduced to reduced graphene oxide (RGO) due to phenol and adhesive phenol on the surface of RGO. The tensile strength of the produced GO/PR nanocomposite fibers was significantly enhanced owing to the uniformly dispersed and oriented RGO nanosheets. Additionally, the ultraviolet protection factor of the highly aligned GO/PR nanocomposite fibers is about 8 times than that of the pure PR fiber. Moreover, the dielectric properties of as-prepared GO/PR nanocomposite fibers also exhibit a tunable performance when change the dispersion of RGO in PR matrix. This adjustable properties suggests an effective method to prepare controllable graphene-based nanocomposites fibers with high performances and novel functional characteristics.

Thursday, 22/Aug/2019 2:12pm - 2:24pm

Abstract ID: 599 / FTF-2: 2

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Metal oxide, carbon, nitrides etc based thins Films

Keywords: TiO₂, CuO, Heterostructures, Thin Films, Gas Sensing

CuO/TiO₂ p-n thin film nanoheterostructures for gas sensing applications

**Katarzyna Ewa Zakrzewska¹, Wojciech Maziarz¹, Marta Radecka², Michał Mazur³,
Damian Wojcieszak³, Danuta Kaczmarek³**

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CuO/TiO₂ represents one of the most promising p-n heterostructures for gas sensing. Recently, Park et al. [1] demonstrated enhanced electrical resistance changes to 0.1-5 ppm of H₂ at 300°C for the multiple-networked TiO₂-decorated CuO nanorod films. In our contribution, we demonstrate CuO and CuO/TiO₂ thin films deposited consecutively by reactive sputtering without breaking a vacuum. Cross-sectional scanning electron microscopy SEM image indicates a growth of fibres perpendicular to the Si substrate (Fig.1). Elemental mapping allows to visualize the interface between CuO and TiO₂ layers (Fig.2). Bi-layered heterostructures synthesized on special gas sensor substrates with precisely defined interdigital electrodes were tested towards NO₂ detection over the low concentration range from 200 ppb to 20 ppm. The aim of this study was to prove that protecting the CuO layers with TiO₂ could allow us to achieve better stability of gas sensing signals and to increase the sensor responses.

Fig.1 SEM cross-sectional image of CuO/TiO₂ Fig.2 Elemental mapping of CuO/TiO₂ thin thin film film

Key Words: TiO₂, CuO, Heterostructures, Thin Films, Gas Sensing

National Science Centre, Poland UMO-2016/23/B/ST7/00894 is acknowledged.

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Abstract ID: 600

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Metal oxide, carbon, nitrides etc based thins Films

Keywords: acetic acid, gas sensing, p-type, n-type, temperature

Study of p-type and n-type behaviour of fast response-recovery rGO- α -Fe₂O₃ based acetic acid sensor

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rGO- α -Fe₂O₃ nanocomposite is synthesized by hydrothermal method for detection of acetic acid vapours. Presence of acetic acid vapors in excess limit can be detrimental for health. The graphene-based nanocomposite is used here for the first time for acetic acid fumes detection. This graphene based thin film composite performs sensing at lower temperature compared to state of the art, which will allow detection of vapours of acetic acid at a lower temperature and minimal time compared to previous reported work. Additionally, the composite showed a p-type to n-type behavior transition. The recovery time of the sensor is much better in p-type while the response time is better in case of n-type. Presence of graphene facilitated lower temperature, fast response sensing of gas molecules. The thin film nano-composite also showed high selectivity towards acetic vapours compared to other analytes, as well as a good stability with change in humidity is obtained. This nano-composite was previously utilized for room temperature CO gas sensing in our earlier work. Here, for the first time this nanocomposite based thin film is utilized for acetic acid vapour sensing. This, highly sensitive acetic acid sensor can be highly beneficial for industries, as well as chemical laboratories.

Abstract ID: 601

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Electrochemical Supercapacitors

Keywords: Opal, Macropores, Nano, Energy Storage

High Voltage Energy Storage Device

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The possibility of creating high-voltage devices for storing and converting energy collected from tens of thousands of supercapacitors is being considered. To improve their performance in electrocatalytic oxygen reduction and reduce the volume of an assembly element, three-dimensional ordered macroporous frameworks constructed of thin porous walls are used to enrich accessible active centers and reduce mass and electron transfer paths. For this purpose, the method of surface coating is used. Synthesis involves the packing of silica nanospheres into an opal surface coating, its carbonization and the removal of templates. Experiments have shown satisfactory characteristics of both ordered macropores in fast mass transfer and thin layers of carbon in fast electron transfer, as well as sufficiently large surface areas to accommodate active objects.

Abstract ID: 602

Symposium 2: Functional Composite Materials (FCM)

Invited Talk

Topics: Fiber reinforced Composites

Keywords: Fiber-Reinforced Composite, Wind Turbine, Pyrolysis Property, Reaction-to-fire Property, Fire Evolution

Developments of Fiber-reinforced Composites Applied in Wind Turbines and Their Thermal and Fire Safety Issues

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Developments and classifications of various types of fibers reinforced composites that are applied in the productions of blades and nacelles of wind turbines were generally reviewed. The properties, compositions, structures and manufacturing processes of glass fibers and carbon fibers reinforced composites including polymer matrices were addressed. Updated applications of basalt fibers, natural fibers (sisal, flax, hemp and protein) in reinforcing resins and using for wind turbines were prospected. To assure long-term effective services of these composites in wind energy, thermal and fire safety issues can not be neglected since there are diverse heat and fire sources practically. Typical thermal environments and fire scenarios were discerned based on real-scale accidents. Pyrolysis courses and properties of typically used fibers-reinforced composites were summarized. Flammability hazards and reaction-to-fire properties of composites were first characterized and assessed. When exposed to potential heat and fire sources, the roles of these composites in initiating and propagating irresistible fires and related influential factors were figured out based on representative fire cases. Evolution patterns, behaviors, properties and mechanisms of such special fires were preliminarily explored and deduced. Based on above observations and findings, requirements for fire safety issues of these materials were proposed. Flame retardant and fire proof solutions were developed. This study provides future insights of establishing thermal and fire safety criteria for wind turbines.

Abstract ID: 603

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: superhydrophobic, nanoparticle, blood repellent

Elastic Superhydrophobic and Photocatalytically Active Films used as Blood Repellent Dressing

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Superhydrophobic surfaces have been extensively studied in various fields because of their great potential to improve people's lives. However, the easily damaged micro/nano structures and the simplified function have greatly limited the practical applications of superhydrophobic surface. As a cheap and eco-friendly material, the current available silicone rubber (PDMS) is extensively used in various areas because of its low surface energy and flexibility. Here, we have proposed to use PDMS crosslinker modified TiO₂ nanoparticles (or some other metal-oxide photocatalysts) to crosslink PDMS, a flexible superhydrophobic surface with photocatalytic activity. The surface presents much better stability than traditional fragile superhydrophobic surface when it is deformed. After many times of bending, the superhydrophobicity can be perfectly maintained. This can be attributed to the recovery of microstructures after external forces working on the surface. At the same time, benefiting from the photocatalytic property, the surface can not only be used to resist contamination of chemicals but also be efficient for purifying solvents with different surface energies. The flexible superhydrophobic surface also presents blood repellent properties making it have great potentials to be used in blood transmission processes.

Wednesday, 21/Aug/2019 5:39pm - 5:51pm

Abstract ID: 604 / FC: 9

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Photocatalysis

Keywords: Dye photo-degradation, Electron donors, Metal–organic frameworks, Photocatalysis, Water reduction.

Concurrent Photocatalytic Hydrogen Generation and Dye Degradation Using MIL-125-NH₂ under Visible Light Irradiation

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The impact of different transition metal-based co-catalysts toward photocatalytic water reduction when they are physically mixed with visible-light active MIL-125-NH₂ is first systematically studied. All co-catalyst/MIL-125-NH₂ photocatalytic systems are found to be highly stable after photocatalysis, with the NiO/MIL-125-NH₂ and Ni₂P/MIL-125-NH₂ systems exhibiting high hydrogen (H₂) evolution rates of 1084 and 1230 $\mu\text{mol h}^{-1} \text{g}^{-1}$, respectively. Second, how different electron donors affect the stability and H₂ generation rate of the best Ni₂P/MIL-125-NH₂ system is investigated and it is found that triethylamine fulfils both requirements. Then, the electron donor is replaced with rhodamine B (RhB), a dye that is commonly used as a simulant organic pollutant, with the aim of integrating the photocatalytic H₂ generation with the degradation of RhB in a single process. This is of supreme importance as replacing the costly and frequently toxic electron donors with hazardous molecules present in wastewater makes it possible to oxidize organic pollutants and produce H₂ simultaneously. This is the first study where a metal–organic framework (MOF) system is used for this dual-photocatalytic activity under visible light illumination and the proof-of-concept approach envisions a sustainable wastewater remediation process driven by the abundant solar energy, while H₂ is produced, captured and further utilized.

Wednesday, 21/Aug/2019 6:24pm - 6:36pm

Abstract ID: 605 / FCM: 13

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Theoretical/Modelling/Computer Simulations Of Functional Materials

Keywords: Porous media, Piezoelectric actuation, Homogenization, Peristaltic pump, Computer simulation

Multiscale modelling of Piezoelectric Porous Architectures for design of smeared peristaltic fluid pumps

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Fluid transport in porous materials can be assisted by the fluid-structure interactions due to actuators distributed in the skeleton, so that smart devices create periodic structures which may be modified in the sense of the functional grading. To explore functionality of such metamaterial structures, we develop computational tools based on the multiscale homogenization approach. We consider elastic composites with distributed piezoelectric actuators and electrode circuits [1]. The computational models arise from the homogenization of the fluid-structure interaction problem. In this way, local cell problems are obtained which provide characteristic responses of the microstructures with respect to macroscopic strains, fluid pressure and electric potentials. Although the deformations are assumed to be small, the macroscopic nonlinearity of the device is captured using the first order expansions of the homogenized coefficients with respect to macroscopic variables. For this, the sensitivity analysis approach is employed [2]. As an optional feature of the smart devices, distributed valves are involved which strongly influence the macroscopic permeability of the material. For this, a homogenized model of the contact problem was developed. We present examples of microstructures and results of the simulations as the proof of concept aimed at designing smeared peristaltic pumps in a bulk medium. The computational tools are intended for subsequent two-scale design optimization [3] of local microarchitectures according to objectives of the macroscopic functionality.

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Abstract ID: 606

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Invited Talk

Topics: Bio-inorganic nanomaterials

Keywords: Nanophosphors, Photodynamic Therapy

Rare earth-doped nanophosphors: Synthesis and novel applications in nanomedicine

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The role of rare earth (RE)-doped YAG (Y₃Al₅O₁₂) nanophosphors on the development of novel biological applications in nanomedicine and bionanotechnology is reviewed in detail. Luminescent nanoparticles and photosensitizer (PS) conjugates capable of X-ray photodynamic therapy (X-PDT) are a research focus due to their potential applications in cancer treatment. Combined with X-PDT, appropriate imaging properties of a GAG (Gd₃Al₅O₁₂) nanoscintillators are suitable for theranostics of deep lying tumors. For these applications, special emphasis will be taken on the different synthesis techniques that are crucial to obtain YAG or GAG nanophosphors with different rare earth-doping in order to control their physical properties (tunable photoluminescence) covering a wide range (from UV to IR) of the electromagnetic spectrum. The present work details the progress of YAG and GAG based nanophosphors with properties useful for biomedical applications such as subtissue nanothermometers, X-Ray mediated photodynamic therapy (X-PDT) for cancer treatment and finally the use of YAG:RE nanoscintillators for radiation dosimetry devices. Ultimately, energy-efficient optoelectronic devices such as solid state white-emitting lamps will also be reviewed.

Thursday, 22/Aug/2019 3:15pm - 3:27pm

Abstract ID: 607 / FLNM-3: 7

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Spectroscopy studies of low dimensional, nano and 2D materials Carbon Based materials

Keywords: Transition Metal Dichalcogenides, Phase Change, MoTe₂, Ionic Liquid, Raman

Reversible 2H to 1T' Phase Change in Monolayer to Bulk MoTe₂ by Ionic Liquid Gating

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Transition metal dichalcogenides (TMDs) exist in various crystal structures with semiconducting, semi metallic, and metallic properties and the dynamic control of these phases is of immediate interest for next generation electronics such as phase change memories.¹ Out of the TMDs, MoTe₂ is attractive for electronic applications because it has the lowest energy difference between the semiconducting (2H) and semi-metallic (1T') phases which makes the MoTe₂ phase change feasible by electrostatic doping.^{2,3} Here we report reversible, electrostatic phase change of MoTe₂ in all thicknesses of MoTe₂, ranging from the monolayer case to effective bulk (60nm), using an ionic liquid electrolyte at room temperature and in air. We find consistent evidence of a reversible 2H-1T' transition using in-situ Raman spectroscopy where the phase change occurs in the top-most layers of the MoTe₂ flake. We find a thickness dependence on the transition voltage that shows higher voltages are necessary to drive the phase change for thicker flakes. We also see evidence of electrochemical activity during the gating process by observation of Te metal deposition. This indicates the formation of Te vacancies which has been shown to lower the energy difference between the 2H and 1T' phase⁴, potentially aiding the phase change process. Our work demonstrates the feasibility of MoTe₂ phase change electronics by moving past the necessity of monolayer devices and allowing for transition voltage tuning by thickness control.

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Thursday, 22/Aug/2019 11:00am - 11:12am

Abstract ID: 608 / FLNM-2: 1

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Applications of low dimensional, nano and 2D materials

Keywords: Hydrogen, photocatalysis, metal organic frameworks (MOFs), 2D materials

2D metal free co-catalyst/metal organic framework hybrid materials for visible light photocatalytic hydrogen production

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Hydrogen is a clean and renewable energy carrier and is considered as the ideal candidate for future mobile and stationary applications due to its clean burning. Hydrogen production via photocatalytic water splitting upon visible light irradiation has been widely studied since it is an earth-abundant, nontoxic and environmentally friendly method. Until now, different materials such as metal oxides, metal sulfides, graphene oxide and graphitic carbon nitride, have been developed as visible light responsive photocatalysts. Metal organic frameworks (MOFs), which are composed of metal ions/clusters connected by organic linkers, represent a promising class of solid crystalline materials for photocatalytic applications due to their advantageous properties such as large surface area, high porosity and optical properties. By tuning the metal clusters or bridging organic ligands, the light absorption of MOFs can be optimized, and desired charge transfer mechanism can be observed.^{1,2} For an efficient electron-hole separation, MOFs are generally combined with co-catalysts, which are based on noble or non-noble metals. Less attention has been paid on metal-free co-catalyst, which are cheaper and more earth-abundant.³ 2D materials such as graphene and others have received great attention in photocatalytic water splitting, and due to their intriguing electronic properties, they are considered as good candidates for the photocatalytic generation of hydrogen when are combined with MOFs. In this lecture, I will present our latest results on using visible light responsive MOFs combined with a plethora of different 2D materials and provide mechanistic insights on the performance of each photocatalytic system using photoluminescence, transient absorption spectroscopy and DFT calculations.⁴

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Thursday, 22/Aug/2019 3:36pm - 3:48pm

Abstract ID: 609 / FTF-2: 9

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Optical, electrical and magnetic properties of thin films

Keywords: organic thin films, magnetic behavior, photoconductivity, liquid crystals

Functional materials derived from exceptionally stable π -delocalized radicals

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Open-shell organic systems are becoming increasingly important structural elements in advanced materials for applications in molecular electronics, energy harvesting, memory and energy storage, and spintronics. In this context, we have been investigating thin films of supramolecular assemblies of stable π -delocalized radicals, such as 6-oxoverdazyl and benzo[e][1,2,4]-triazinyl (I). We have developed access [1] to derivatives of I with new molecular architectures [2] and to liquid crystals exhibiting discotic (Colh) [3] and bent-core (SmA) phases [4]. SQUID measurements revealed that the discotic materials exhibit magnetic behavior that is structure-dependent and the spin-spin interactions range from antiferromagnetic to ferromagnetic in the solid phase. Photoconductivity studies demonstrated that the hole mobility is about $\mu \approx 1.3 \times 10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ in the fluid Colh phase [3]. Films formed by molecules with new architectures of the cores (planar geometry and multi-spin molecular cores) give rise to appearance of new liquid crystalline phases, modulation of magnetic behavior as function of the phase structure, and improvement of mobility of the photoinduced charges.

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Abstract ID: 610**Symposium 3: Functional Catalysis (FC)****Oral Presentation**

Topics: Photocatalysis

Keywords: Photocatalysis, Spectroscopic methods for structural characterization, Fundamentals of catalysis

Tracing the active atomic sites in photochemistry with soft X-ray resonant inelastic X-ray scattering

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Active atomic sites in photochemical processes are a central conceptual approach onto which governing principles of rate and selectivity are based. The optical radiation is behind both the desired processes of charge separation and photochemical heterogeneous catalysis but also requires efficient mechanisms of photoprotection to shut off unwanted radiation damage. Since they are highly dispersed within the molecular moiety itself, but even so in the typical solvation environment, their observation requires ideally exquisite selectivity of the orbital based valence electronic structure at these active sites in real time only possible with femtosecond and picosecond FEL and Synchrotron soft X-rays. Having established the fingerprints of time resolved resonant inelastic X-ray scattering (RIXS) recently [1,2] a series of deep atomic insights to photochemical processes has been achieved: For saturatively coordinated transition metal complexes in heterogeneous catalysis, the competition between ultrafast intramolecular spin relaxation and solvent induced scattering in ligand substitution is established [3,4]. For photo-driven charge separation in spin-cross over complexes the additional importance of $s - \pi$ valence interaction is established [5,6,7]. Finally, the highly selective bond elongations in photoprotection through tautomerization has been observed and quantified [8,9].

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Abstract ID: 611

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Advances in Deposition Techniques for thin films

Keywords: low temperature growth, local nitrogen plasma, GaN, MOCVD

Low temperature Growth and Characterization of GaN Films via Local Nitrogen Plasma Metalorganic Chemical Vapor Deposition

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GaN materials have been well developed for its applications on optoelectronic devices such as light emitting diodes, laser diodes and electronic devices such as high-electron-mobility transistors. The most common method to growth high quality GaN materials in industry is Metalorganic chemical vapor deposition method, which is usually operated at a high temperature of 1000°C or above. During growth procedure, a large amount of ammonia must be transported into the MOCVD reactor to obtain a high V/III ratio of several thousands to guarantee high quality of the grown GaN materials. A new growth technology which allows low temperature growth with low consumption of the raw materials should be benefit to reduce the material growth cost and related pollutions and even explore novel GaN device applications grown on low cost glass substrate or even flexible substrates.

Plasma is considered to a powerful technology to realize the above projects, which can provide efficient energy for adsorbed atoms to mobile to low energy sites for high quality films growth. Also, plasma can be employed to ionize molecule nitrogen to atomic nitrogen, which is considered to substitute ammonia as nitrogen precursor for GaN growth. However, plasma technology is not so easily to be employed into metalorganic chemical vapor deposition process. The existence of plasma in the growth region will cause the high dissociation of metalorganic precursors and as well as carbon hydrogen radicals, resulting in high gas phase parasitic reaction and high carbon contamination with the quality of grown films highly deteriorated. In the case, remote nitrogen plasma technology was applied to get rid of the above disadvantage. However, the big distance between the plasma generation and growth zone will lead the efficiency of nitrogen ionization decrease a lot, leading a low percentage and low mobile energy of atomic nitrogen, with a low quality GaN films usually obtained by the method.

In the presentation, instead of remote plasma technology, a local nitrogen plasma system has been developed for low temperature GaN MOCVD growth. In this method, a nitrogen plasma was generated in close proximity to the growth region, which will provide enough high efficiency and high energy of atomic nitrogen for GaN growth. The technology can also protect the metalorganic precursor from the localized plasma to minimize its effect on metalorganic radicals, and then eliminate the gas phase parasitic reaction during growth and carbon contamination in the finally films in a great degree. Rather high quality GaN films will then be grown via the local nitrogen plasma MOCVD method. Raman scattering, X-ray diffraction, atomic force microscopy, and photoluminescence will be employed to characterize the structural and optoelectronic properties of the low temperature grown GaN films.

Thursday, 22/Aug/2019 3:00pm - 3:12pm

Abstract ID: 612 / FESC-2: 6

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Lithium Ion Batteries

Keywords: Graphene, Lithium Sulfur Battery, Aluminum-ion Battery

Beyond lithium ion batteries – Opportunities and challenges

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Mobile technologies hinge upon the availability of batteries to support them. The lithium ion battery (LIB) is the workhorse for powering today's mobile devices despite that fact that it was developed in the 1970s, and now lags in its ability to keep pace with the advancements in mobile technologies. In this regard, the lithium sulfur (LSB) battery looks promising due to its reversible and inexpensive energy storage characteristics but unfortunately, the dendrite growth (anode) and shuttle effect (cathode) in a LSB hinder its practical application. New electrolytes for LSBs will be discussed which promote the simultaneous formation of bilateral solid electrolyte interfaces (SEI) on the sulfur-host cathode and lithium anode, thus effectively suppressing the shuttle effect and dendrite growth. The LSBs with new electrolytes exhibit a long-term cycling stability, ultrafast-charge/slow-discharge rates, low self-discharge performance, and a capacity retention of 95% even after a 130 days long storage.

Notwithstanding this progress in LSBs, they still rely on Li metal whose reserves could be depleted in as little as fifty years if the demand for electric vehicles grows as expected. Thus, choosing newer materials beyond Li is imperative for replacing Li battery chemistries. Aluminum, the most abundant metal in the Earth's crust (~8% vs. 0.0065% for Li) displays a three-electron redox reaction compared to the Li one-electron redox reaction. Few layer graphene is a promising cathode material for aluminum ion batteries (AIBs) that use chloroaluminate (AlCl₄⁻) ionic liquids as the electrolyte. A fundamental understanding of interactions between the few layer graphene cathode and the ionic liquid electrolyte is key for realizing the full potential of these systems. Through in situ Raman spectroscopy and density functional theory calculations, we show that the cathode is capable of achieving stage-one intercalation within the operating voltage window, leading to improved cell performance.

Key Words: Graphene, Lithium Sulfur Battery, Aluminum-ion Battery

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Abstract ID: 613

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Structural, electrical, mechanical and optical of low dimensional, nano and 2D-layered oxides, nitrides and sulfides

Keywords: Liquid crystals, LCD materials, dielectric anisotropy, optoelectronics

High dielectric anisotropy fluid materials derived from boron clusters

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Liquid crystal displays (LCD) use thin films of polar anisotropic fluid materials (polar liquid crystals) to achieve electric field-induced optical switching. The critical voltage, V_{TH} , needed for such an electrooptical effect depends on $(\Delta\epsilon)^{-1/2}$. Therefore, there is a continuous search for new polar derivatives to formulate LCD materials with dielectric anisotropy $(\Delta\epsilon)$ as a molecular design parameter. A series of nematic and smectic zwitterions 1–4 incorporating the [closo-1-CB9H10]- and [closo-1-CB11H12]- clusters was investigated as potential high dielectric anisotropy $(\Delta\epsilon)$ additives for nematic hosts. The compounds were characterized by thermal, optical and dielectric methods in thin film electro-optical cells. The pyridinium fragment in the antipodal position in the series 1[m,n] and 2[n] gives rise to a longitudinal dipole moment of about 12 D, which results in $\Delta\epsilon$ values as high as 60. Some of the esters 3[n] exhibit nematic behavior and form stable solutions in a nematic host up to 5 mol %. The extrapolated values of $\Delta\epsilon$ for 3[n] zwitterions are 21 (for the least polar, $\mu = 12$ D) and 70 for the most polar ($\mu = 70$ D). Derivatives 1[m,n] exhibit exclusively smectic behavior. Experimental results are augmented with DFT calculations and analyzed using the Maier-Meier relationship.

Abstract ID: 614

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Nanostructured and Architecturally Designed Coatings, Smart Surfaces

Keywords: Ta-Based, thin films, nano-porous, biocompatibility

Preparation and Characterization of horizontally-aligned porous Ta, TaON, and Ta₂O₅ films synthesized by co-sputtering and de-alloying approach

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In this study, Ta-Cu films were first prepared using reactive co-sputtering. After deposition, the films were annealed, and Cu was etched away to form nano-porous structures. The films were characterized using four-point probe, nano-indentation, XRD, and SEM. The results showed that the porous structure of these films were horizontally-aligned. The nano-porous samples were then treated using rapid thermal annealing (RTA) process to form oxide and oxynitride with similar roughness. At final, these nano-porous samples are tested for their biocompatibility and viability using MG-63 cells. According to the results obtained from biocompatibility and MTS assay testing, it was found that the oxynitride showed the poorest results. Furthermore, these porous films show unique mechanical properties.

Abstract ID: 615

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Ceramic based composites

Keywords: Bi₂O₃; PbO; Mechanical properties; Ceramics; Sintering

Effects of Bi₂O₃ addition on the Mechanical properties of PbO ceramics in Lead-cooled fast reactor

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Effects of Bi₂O₃ addition on the mechanical properties of PbO ceramics were studied in this research. Specimens with different Bi₂O₃ concentration were fabricated and sintered at 620°C. Mechanical properties such as density, hardness, and flexural strength were measured. Results showed that fine microstructure and mechanical properties would be obtained with the 3wt.% Bi₂O₃. The X-ray diffraction analysis revealed that solid solution formation took place in the 3wt.% Bi₂O₃-97wt.% PbO ceramic. The hardness and the flexural strength is 267% and 77% higher than that of 100wt.% PbO respectively. The toughening mechanisms of Bi₂O₃ are mainly attributed to grain growth due to solid solution formation.

Abstract ID: 616**Symposium 1: Functional Biomaterials and Biosensors (FBB)****Oral Presentation***Topics:* Regenerative Medicine*Keywords:* Bone, Electrospun, Fracture Healing, Scaffold**Phosphodiesterase Inhibitor and Connective Tissue Stimulating Drugs Loaded Nanofibrous Scaffolds for Enhanced Bone Fracture Healing****Isra Hussein Ali¹, Islam Ahmed Khalil^{1,2}, Ibrahim Mohamed El-Sherbiny¹**¹Zewail City of Science and Technology, Egypt; ²Misr University for Science and Technology; igalal@zewailcity.edu.eg

Normal fracture healing without scars is considered to be a complicated and challenging process. Bone healing is affected by a number of factors; the most important of them is the presence of adequate blood supply to the damaged tissues. Bone healing starts with the hematoma phase, which involves clot formation followed by platelet degranulation, and finally the release of growth factors at the fracture site. A 3D electrospun nanofibrous matrix was fabricated as using electrospinning technique using biocompatible and biodegradable materials, mainly polylactic acid (PLLA), to be used for the purpose of tissue regeneration and healing. The 3D matrix was designed to act as both a fracture healing scaffold and a single-dose controlled drug delivery system for some healing agents such as Phenytoin and Sildenafil citrate which were selected as model drugs for this study. Phenytoin, an antiepileptic drug, has been proven to have a positive effect on healing process through the acceleration of tissue epithelization and granulation, reduction of inflammation and the bacterial load, and facilitating the nerve regeneration. Sildenafil, an inhibiting phosphodiesterase-5 enzyme, is primarily used as a treatment of men's erectile dysfunction (Viagra®). It also stimulates angiogenesis that plays an important role in fracture healing through its upregulation of pro-angiogenic factors known as vascular endothelial growth factor (VEGF). In addition, Sildenafil showed increased callus formation through the cysteine rich protein(CYR61) pathway. Highly porous PLLA multi-layered scaffold loaded with previously mentioned drugs were developed successfully showing fibers diameter ranging from 350-500 nm. In Vitro drug release profile showed that the produced nanofibers were capable of delivering the drugs in controlled manner along 3 weeks. Biodegedability test showed that the scaffold had the capability of maintaining more than 70% of its original weight after 3 weeks. Biocompatibility test showed that both the loaded and unloaded nanofibers not only helped in surviving the tested cells but also in enhancing the cell proliferation. This was also detected through investigating the cell attachment on the nanofibers under the scanning electron microscope. Finally, the in Vivo model using rabbits and the histology experiments showed the ability of the drug loaded scaffolds to heal the bone fracture partially after 14 days while completely after 28 days compared to the control groups. DEXA revealed significant increase in bone mineral density for the defect treated with dual drug-loaded scaffold in comparison with non-medicated ones after 28 days. Therefore, the electrospun drug-loaded scaffold could be considered to be a promising treatment for complicated bone fractures through targeting different phases in the healing process.

Thursday, 22/Aug/2019 8:15am - 8:30am

Abstract ID: 617 / FCM-2: 2

Symposium 2: Functional Composite Materials (FCM)

Invited Talk

Topics: Green Composites

Keywords: SWCNT, PPy, PhC2Cu, PEDOT, TE nanocomposites

Carbon nanotube-based composites and their thermoelectric performance

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Thermoelectric (TE) materials are becoming increasingly significant in academia due to their functionality in the direct conversion between heat and electricity. A highly efficient and economical way to fabricate materials with high TE performance and potential application is the formation of hybrid or composite structures from organic and inorganic components.^{1–5} Therefore, we prepared three types of flexible single-walled carbon nanotube (SWCNT)-based TE composites (polypyrrole/SWCNT (PPy/SWCNT) nanocomposites,^{1,2} copper-phenylacetylide/SWCNT (PhC2Cu/SWCNT) nanocomposites,³ and poly(3,4-ethylenedioxythiophene)/SWCNT (PEDOT/SWCNT) nanocomposites⁵) by utilizing the high electrical conductivity of SWCNT and varying organic materials.

The PPy/SWCNT cable-like nanocomposites possessed large-area, super flexibility (minimum bending radius < 0.6 mm), stretchability and mechanical stability, affording greatly enhanced TE performance with the maximum power factor of $21.7 \pm 0.8 \mu\text{W m}^{-1} \text{K}^{-2}$.

As for the PhC2Cu/SWCNT nanocomposites, an unusual mechanochromic luminescence phenomenon from bright green to dark red is clearly observed after grinding the PhC2Cu crystalline nanobelts. The PhC2Cu/SWCNT composites displayed high mechanical flexibility and excellent TE performance. The maximum power factor at room temperature reached as high as $200.2 \pm 10.9 \mu\text{W m}^{-1} \text{K}^{-2}$, opening an avenue to fabricate novel organic–inorganic TE composite materials using organometallic coordination compounds.

The PEDOT/SWCNT) nanocomposites were prepared by dynamic 3-phase interfacial polymerization and subsequent physical mixing. The SWCNT content greatly affected the composite thermoelectric performance. The maximum power factor for the composites reached $253.7 \pm 10.4 \mu\text{W m}^{-1} \text{K}^{-2}$, being one of the highest values for polymer-based thermoelectric composites.

Abstract ID: 618

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biomaterials for Cardiovascular Applications

Keywords: magnetic resonance imaging, nano-sensor, diagnostics, cardiovascular disease, thrombosis

Activatable Gadolinium-Iron Oxide Nanoparticles for Detection and Discrimination of Thrombosis

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The early detection and accurate characterization of life-threatening diseases such as cardiovascular disease and cancer are critical to the design of treatment. Knowing whether a thrombus in a blood vessel is new/fresh or old/constituted, and whether a tumour mass has hypoxia region is very important for physicians to decide a treatment protocol. Non-invasive differentiation between old and fresh thrombi would be of clinical importance to estimate the risk for embolization and the necessity of anticoagulation. Currently, there are a handful of MRI methods for imaging of thrombus, all of which have weakness in their approach and there has been no single imaging agent that can simultaneously detect and grade the age of the thrombus. Here we report the design and development of smart magnetic resonance imaging (MRI) nano-sensors that can not only detect, but also sense and report the stage or progression of cardiovascular diseases such as thrombosis. The nano-sensors are functionalized with binding ligands that target fibrin, a major component of thrombosis; and are able to switch between T1 and T2 signal depending on the age of the thrombus. The nano-sensor exhibits T2 effect in the absence of thrombin (dark signal), while it shows T1 effect in the presence of thrombin (bright signal). Since thrombin enzyme is only present in the fresh/new thrombi and absent in the old/aged ones, the nano-sensor is activated by thrombin and shows T1 effect on the fresh thrombi while it is non-activated and shows T2 effect on the old ones. Our data shows that these MRI nano-sensors are able to image and distinguish between fresh and old thrombi. This is a “one stop shopping” approach where a single imaging agent can be used to identify and classify thrombus throughout the body. The potential use of these nano-sensors is beyond cardiovascular disease and can also be applied for cancer detection.

Abstract ID: 619**Symposium 1: Functional Biomaterials and Biosensors (FBB)****Oral Presentation***Topics:* Biomaterials for hard tissue applications*Keywords:* Porous Silicon, Bone Regeneration, Tissue Engineering**Porous silicon for tissue engineering: spectroscopic studies of dissolution****Pierre-Yves COLLART DUTILLEUL¹, Naveen FATIMA¹, Frédérique CUNIN², Frédéric CUISINIER¹**¹LBN, University of Montpellier, France; ²ENSCM, UMR CNRS University of Montpellier, France; pierre-yves.collart-dutilleul@umontpellier.fr

Porous silicon has a unique combination of properties that makes it a suitable scaffold for tissue engineering. This review focuses on porous silicon (pSi) microparticles as a bioactive scaffold for tissue engineering, which facilitates human cell adhesion and further differentiation, thus providing clues to clinically enhance regeneration. Mapping the kinetics of pSi degradation is essentially important for in vivo applications, in order to adapt biomaterial resorption to tissue formation.

The properties of biodegradation and bioactivity have inverse correlation, as increase in bioresorption decreases its bioactivity by depleting the material fast. We made an overview of available studies following pSi degradation and silicic acid release in relation to time, utilizing spectroscopic techniques, such as Raman spectroscopy, Fourier transformed infrared spectroscopy (FTIR), energy dispersive X-ray spectroscopy (EDX), X-ray photoelectron spectroscopy (XPS), interferometric reflectance spectrometry (IRS) and inductively coupled plasma mass spectroscopy (ICP-MS). We related the results to different microscopic observations. Finally, comparing our research to the current data available on pSi characteristics.

pSi resorption with silicic acid release appeared immediately after implantation with a maximal dissolution in the first 24 hours. Then, the dissolution rate decreased over time. During dissolution, spectroscopic evaluation revealed that a non-crystalline (amorphous) layer appeared at the pSi surface. For non-oxidized particles, surface oxidation could be observed after immersion in aqueous solution, and this oxidation seemed to interfere with dissolution. Still, non-oxidized pSi dissolved at a much faster rate (> 90%) than oxidized pSi in physiological media and the maximum morphological changes occur during the initial hours of incubation. These changes are clearly observed by decrease in film and particle thickness, analyzed by SEM and optical microphotograph. During degradation silicic acid release is accompanied by liberation of hydrogen gas microbubbles out of the solution that can be appreciated by naked eye. Oxidation introduces morphological and compositional changes in the porous structure, resulting changes in the interaction between pSi and aqueous solution. The delayed dissolution of oxidized pSi particles over non-oxidized increases the bioactivity. Moreover, this stability is of immense importance when scaffold is required to withstand corrosive physiological environment for specific period of time before complete dissolution.

Abstract ID: 620

Symposium 2: Functional Composite Materials (FCM)

Invited Talk

Topics: Multifunctional composites

Keywords: Nanocomposites, Laser deposition, Luminescence, Temperature and Gas sensor, Resistive switching.

Multifunctional Properties of CdS:SiO₂ Nanocomposite Thin Films

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CdS:SiO₂ nanocomposite thin films (NCTFs) possessing multifunctional properties were realized by a novel synthesis method involving swapping of targets in pulsed laser deposition system. Targets of CdS and SiO₂ were swapped at a frequency ratio of 2:8 laser pulses/sec. The composition of CdS and SiO₂ in NCTFs was confirmed by x-ray photoelectron spectroscopy analysis and was found as 21:79 which was nearly same as the ratio of incident pulses/sec (i.e. 2:8) on the two targets. The basic characterizations tools viz; glancing angle x-ray diffraction, micro-Raman spectroscopy and selected area diffraction pattern were used to confirm the formation of CdS crystalline phase and transmission electron microscopy were used to visualize the formation of CdS nanocrystals in NCTF systems after annealing. Room temperature photoluminescence (PL) was carried out to study the emissive radiative states present in the systems [1]. Low and high temperature PL were recorded to realize luminescence based wide range (20-560K) temperature sensor with average sensitivity and resolution of the sensor were \square 10⁻² K⁻¹ and 10⁻⁴ K respectively and a maximum relative sensitivity \sim 8.4 % K⁻¹ at 120 K. The developed sensor exhibits almost linear behavior in all cryogenic, physiological, and high temperature ranges [2]. Further, the same set of NCTFs was used to explore the gas sensing properties. For this purpose, the resistances of the films in air and in the presence of reducing gases viz. LPG, H₂, H₂S, NO₂ and CO₂ were measured. The sensor shows highest response for LPG and observed value is \sim 71 % for 1000 ppm at RT with response time and recovery time as 91 s and 140 s respectively. In addition to above two applications, the resistive switching behavior of NCTFs was also observed to develop the non-volatile memory.

Abstract ID: 621 / Poster: 30

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Manufacturing and formation techniques

Keywords: functional microparticles, microfluidics, core/shell structure

Needle based microfluidic formation of double emulsion structure encapsulating multiple cores

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Polydimethylsiloxane (PDMS) microdroplets with multiple cores were fabricated by needle-based microfluidic device. The core-shell structure of microdroplets utilized water-in-oil-in-water (W/O/W) double emulsion template. The shell was made of PDMS and the cores were dyed water, while the outer phase to shear the inner and middle phase was water with surfactant. By tuning the flow rates of inner and middle phases, up to twelve cores could be capsuled inside the PDMS shell. Additionally, the size of the cores could be manipulated either by flow rates or applying various needles combinations with different sizes. The sizes of microdroplets were highly monodispersed both for the overall size and the size of cores. It is always preferred that the microdroplets were generated under dripping flow region. The PDMS microdroplets were thermally cured off-site to form functional microparticles and stored for applications such as encapsulation which can be involved in energy storage and conversion. The needle-based microfluidic device is versatile, reliable and cost-effective.

Abstract ID: 622

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Smart Composites

Keywords: Shape memory, Polyimide, hemiaminal, Hexahydrotriazine, complex geometry

Tough and strong thermoset shape memory polyimides

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Shape memory polyimide composing of excellent toughness, complex geometry and easily shaped will facilitate great potential application in harsh environment, but remains challenging. Herein, we report a new strategy to prepare functional shape memory polyimides via polycondensation of polyimide oligomers with paraformaldehyde. The polyimide hemiaminal dynamic covalent networks (PI-HDCNs) formed at low-temperature have excellent toughness and show dynamic covalent effect, which can further cyclize at higher temperature to produce polyimide poly(hexahydrotriazine)s network (PI-PHTs). The PI-PHTs with a molecular weight of oligomers as low as 8 kg/mol possess superior mechanical properties compared to state-of-the-art high-molecular-weight polyimide and the optimal thermoset achieves tensile strength of 89.7 MPa, elongation ratio of 78%, and toughness up to 69.2 MJ/m³, respectively. The optimized PI-PHTs exhibit high temperature triggered shape-memory effect with shape fixity ratio above 98% and shape recovery value above 90%. The shape recovery ratio of PI-PHTs can be effectively controlled by adjusting the molecular weight of oligomers. Extraordinarily, combining the unexceptionable toughness and dynamic covalent behavior of PI-HDCNs, the block sample, complex geometry and surface micropatterns of shape memory composites can be facilely obtained. These merits are expected to significantly broaden the applications of shape memory polyimides.

Abstract ID: 623

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Metal matrix composites

Keywords: Molecular dynamics, silicon carbide, graphene

Molecular Dynamics Simulation of SiC-Graphene Reinforced Aluminum Hybrid Composites

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Metal matrix composites (MMCs) are nowadays widely used in various areas such as automotive, aerospace and electronics. Moreover, the particle reinforced MMCs are of particular interest because of their excellent mechanical and physical properties [1]. Recently particles of silicon carbide (SiC) were used as reinforcement for aluminum matrix [2,3] which helped in increasing the elastic modulus and tensile strength of the composites. A number of studies have been conducted on SiC particle reinforced aluminum composites (SiC-Al) in the last few decades [4]. All of these studies suggested that the deformation behavior of MMCs is dominated by the reinforcing particles. Experimental studies showed that the mechanical properties of these composites depend on the volume fraction (Vf), size and distribution of the SiC reinforced particles. Though a number of experimental studies have been conducted on SiC-Al composites, still the microstructural changes in these composites have not been understood fully because of the difficulties with in-situ detection using the laboratory apparatus. In this study, the effect of SiC nanoparticle will be studied at the atomic level by using MD approach. For this purpose, the Biovia Materials Studio [5] software will be used for modeling and analysis of the composites. The diameter of the SiC nanoparticle will be taken as 10 Å. Firstly, the pure Al matrix will be modeled for predicting its properties. This will be followed by reinforcing the Al-matrix with varying volume fraction (Vf) of SiC nanoparticle. The Vf will be varied from 0-20% for studying the variation in the properties of the SiC-Al composite. The effect of graphene will be also studied by reinforcing SiC-Al with graphene. The properties of this hybrid composite will be then predicted using the Forcite module of the Biovia Materials Studio [5] software.

Key Words: Graphene, Silicon-carbide, Molecular dynamics

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Abstract ID: 624

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Electrochemical Supercapacitors

Keywords: CuCo₂S₄, MnCo₂O₄, Pseudocapacitance

Synthesis of CuCo₂S₄/MnCo₂O₄ nanorod arrays on Ni foam as binder-free electrode for asymmetric supercapacitor

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Supercapacitors as one of the energy storage devices have greatly excited researchers' interests because they exhibit fast charge/discharge rate, long cycle life, good rate capability and high power density [1,2]. Faradaic pseudocapacitors can offer much higher energy density than electric double-layer capacitors, which is resulted from rich faradaic redox reactions producing pseudocapacitance. Transition metal sulfides for instance nickel sulfide, cobalt sulfide, copper sulfide, and nickel cobalt sulfide exhibit higher capacitance than some transition metal oxides and conductive polymers. Among them, ternary transition metal sulfides have recently been observed to offer better electrochemical performances than binary counterparts due to much richer redox reaction sites and higher electric conductivity as a result of the lower band gap. Little attention is paid on the development of CuCo₂S₄ and its composite electrode materials [3].

In this work, CuCo₂S₄/MnCo₂O₄ nanorod arrays were grown on Ni foam by a three-step method. CuCo₂O₄ nanorod arrays were grown on Ni foam by a hydrothermal method, and then transferred into CuCo₂S₄ by reaction with S²⁻ under the hydrothermal condition. After that, MnCo₂O₄ nanosheets were coated on the surface of CuCo₂S₄ nanorod arrays by electrodeposition. The as-prepared CuCo₂S₄/MnCo₂O₄ nanorod arrays on Ni film were used as a binder-free electrode for the assemble of a high-performance asymmetric supercapacitor. The specific capacitance of as-prepared CuCo₂S₄/MnCo₂O₄ electrode can reach 4050 F g⁻¹ at a current density of 1 A g⁻¹. The asymmetric supercapacitor composed of CuCo₂S₄/MnCo₂O₄ electrode as positive electrode and activated carbon (AC) as negative electrode exhibits a high energy density of 44.5 Wh kg⁻¹.

Abstract ID: 625

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Advances in the Synthesis and Characterization of low dimensional, nano and 2D materials

Keywords: Dyeing wastewater; Flocculation; Nanocellulose; TEMPO-NaClO-NaBr

Preparation and Properties of Nanocellulose-based Flocculant

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In order to effectively treat industrial printing and dyeing wastewater, sodium iodate is used to oxidize the hydroxyl groups at the C2 and C3 positions of the cellulose to aldehyde groups, and then further oxidized to cellulose dicarboxylate with sodium chlorite to prepare a flocculant. As a comparison, a nanocellulose flocculant selectively oxidized at the C6 position was prepared using the TEMPO-NaClO-NaBr system. The flocculation performance of methylene blue solution was investigated. The results showed that the flocculant dosage was 2.0 g/L and the pH value was 6. When 250 mg/L methylene blue dye wastewater was treated, the decolorization rate of cellulose-based flocculant prepared by TEMPO/NaClO/NaBr oxidation system was 97.18%, and the adsorption amount was 120.78 mg/g. The decolorization rate of dicarboxycellulose obtained by continuous oxidation of NaIO₄-NaClO₂ was 79.88%, and the adsorption amount was 99.21 mg/g. It is more advantageous to adopt a TEMPO/NaClO/NaBr system than a cellulose-based flocculant prepared by continuous oxidation of NaIO₄-NaClO₂.

Abstract ID: 626

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Electrochemical Supercapacitors

Keywords: MoO₃, supercapacitor, Ag

One-dimensional MoO₃ Modified by TiO₂ and Ag Nanoparticles for Supercapacitor with Enhanced Electrochemical Performance

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In the past years, the practical application for MoO₃ has been limited due to the poor electrical conductivity, a low specific capacitance and slow faradaic redox kinetics of MoO₃. How to improve the conductivity of MoO₃ and enhance the transfer of electrons and ions has been one of the most attractive topics in scientific fields. In order to solve these problems, there are two effective methods have been widely studied include coupling with other nanoparticles to increase its specific area and introducing good conductivity materials to improve its conductivity. In our previous work, the strategy for grown of TiO₂ nanoparticles on MoO₃ nanobelts with higher specific area has been developed and has higher electrochemical performance. Based on the past work, the specific area and the conductivity of MoO₃ electrode have been further improved by introducing Ag nanoparticles. The most important is that a facial strategy for the Ag nanoparticles grown on MoO₃ nanobelts has been developed, which has several advantages, including environmentally friendly, low cost and great enhancement for nanocomposites in electrochemical properties. On the basis of the combining results from transmission electron microscope and scanning electron microscope, the as-prepared nanocomposite has nanobelt-like structure and Ag nanoparticles uniformly distributed onto MoO₃ nanobelts. The electrochemical results showed the composite has enhanced specific capacitance, which is 3 times than pure MoO₃ at the same test condition. The improved electrochemical properties could be attributed to the increment of specific surface area and superior conductivity. This work would not only promote the study about MoO₃-based electrode materials in supercapacitors, but also extended to other transition metal oxides with similar structures.

Abstract ID: 627

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

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

Keywords: all optical modulator, 2D materials, TMDCs, plasmonics, 2D printer

All Optical Plasmonic WSe₂ Based Modulator

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Two-dimensional (2D) transition-metal dichalcogenides (TMDCs) are characterized by unique optoelectronic properties including tunable emission [1], quantum confinement [2] and strong exciton binding energies [3], making them versatile platform for on chip integrated photonic devices ranging from laser [4], photodetector [5] and modulator [6]. However, the optical response of the 2D materials can be modulated by tuning their carrier density via electrical or optical means that modify their physical properties (e.g., PL, transmission or nonlinear absorption) [7]. Hereby, we demonstrate an integrated all-optical modulator in the near infrared region based on a WSe₂ monolayer transferred by 2D-printer technique [8] on top of a plasmonic slot. The modulation is obtained by the interplay of the plasmonic mode confinement in the nano-gap structure and near-field coupling with the WSe₂. The guided mode within the plasmonic slot substantially intensifies the light-monolayer interaction and concurrently tunes the WSe₂ carrier concentration. The excitonic absorption efficiency can be further tailored by the laser pump fluence, achieving a pronounced modulation for optical telecommunication wavelengths. This device can be potentially used in integrated photonic circuit as compact all-optical high-speed modulator and as nonlinear module in photonic neuromorphic computing.

Abstract ID: 628

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Applications of Composites

Keywords: Ferrites, Nano, Energy Storage, nanocomposites

Magnesium ferrite/polyvinyl alcohol (PVA) nanocomposites: fabrication and characterization

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Terbium doped magnesium spinel ferrites ($Mg_{1-x}Tb_xFe_2O_4$) and PVA/ $Mg_{1-x}Tb_xFe_2O_4$ composites having composition $x=0.12, 0.14, 0.16, 0.18$ were synthesized using micro-emulsion method and in-situ polymerization technique respectively. The structural properties were demonstrated using X-ray diffraction (XRD) and Fourier transform infra-red spectroscopy (FTIR). XRD analysis confirmed the fabrication of small concentration of Terbium into the spinel lattice whereas FTIR exposed the developed interactions between ferrite nanoparticles with polyvinyl alcohol matrix. The peaks obtained in both the above characterization techniques quite matched with those as reported in the literature and confirmed the formation of resulting nanocomposites. The dielectric and resistivity analyses were performed by determining dielectric parameters and current-voltage measurements. The values of dielectric constant, dielectric loss and $\tan \delta$ were inversely proportional to the frequency under applied electric field at room temperature but become constant at higher frequency values. The lower values of dielectric constant of terbium incorporated magnesium ferrite polymer composites ($MgFe_2O_4/PVA$) are because of hindrance in electron exchange mechanism created by lockup among iron and terbium ions. The resistivity values of all the composites were found from $2.5 \times 10^9 \Omega cm$ to $18.8 \times 10^9 \Omega cm$ which showed a non-linear behavior.

Wednesday, 21/Aug/2019 6:27pm - 6:39pm

Abstract ID: 629 / FBB-2: 13

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biomaterial surfaces

Keywords: dehydrated, carbon, methylene blue, drug, adsorption

functionalized dehydrated carbons from date palm leaflets for pollution control of organic compounds

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Acidic dehydrated carbon (DC) was prepared from date palm leaflets via sulfuric acid dehydration at 200 °C. using amide coupling process. Dehydrated carbon (DC) was surface functionalized using ethylene diamine and ethylamine to produce basic dehydrated carbon (BDC) and hydrophobic dehydrating carbon (HDC), respectively. Surface characterization was carried out for these carbons including surface area, SEM, EDX, XRD, pH_{zpc}, zeta potential, FTIR, TGA and surface functionality. Surface area was found to be almost 90 times higher for activated carbon than for dehydrated carbons. FTIR and TGA in addition to surface functionality tests showed a successful surface functionalization via chemical bonding. In a comparison with a commercial activated carbon (AC), these carbons were tested for the removal methylene blue and some pharmaceuticals (chlorpheniramine, Ibuprofen, levofloxacin and atorvastatin) in terms of pH, contact time, concentration and column studies. BDC and HDC possess lower surface area than DC due to surface functionalization. Commercial AC showed slow removal processes compared with dehydrated and functionalized dehydrated carbons. Sorption kinetics data followed well pseudo second order model with activation energy falling within physical adsorption processes. Equilibrium sorption data were tested for Langmuir isotherm and were found to fit very well unlike the Freundlich model. Adsorption capacity showed that HDC shows the fastest adsorption with the largest uptake of methylene blue and other drugs regardless of its very low surface area. HDC with surface area 5.4 m²/g shows better adsorption properties of methylene blue than AC (1056 m²/g). Dominant forces of adsorption varied from carbon to another. Thermodynamic parameters showed that the adsorption processes are spontaneous and endothermic with ΔH_0 falling within physical adsorption processes. column studies showed better performance on functionalized carbons than activated carbon.

Thursday, 22/Aug/2019 12:24pm - 12:36pm

Abstract ID: 630 / FCM-3: 8

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Bio-inspired design of composites

Keywords: wellbore stability, biopolymer, encapsulators, water-based drilling fluids, chemical strengthening

Enhancing wellbore stability of water-based drilling fluid using a novel catechol-chitosan biopolymer encapsulators

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The problem of wellbore stability has a marked impact on oil and gas exploration and development in the process of drilling. Effective physical plugging and chemical cementing is the key measure to guarantee the wellbore stability which is the results of both physical and chemical factors. Marine mussel proteins can adhere and encapsulate firmly on deep-water rocks, providing inspiration for solving borehole stability problem and this ability comes from catechol groups. In this paper, a novel biopolymer, synthesized with chitosan and polymers containing catechol structure by Schiff base-reduction reaction method, was developed as an encapsulator in water based drilling fluids (WBDF). It was characterized by Fourier transform infrared spectrum analysis, nuclear magnetic resonance, and gel permeation chromatography. In addition, the chemical enhancing wellbore stability performance of WBDFs containing different encapsulators were experimentally investigated and compared by tension shear strength test, shale hot-rolling dispersion experiment, uniaxial compression test and scanning electron microscope (SEM) analysis. The results showed that there are aromatic ring structure, amines and catechol groups in catechol-chitosan biopolymer molecule, which can chelate with metal ions and form stable covalent bonds. The relative molecular weight is about 30,000. The high shale recovery rate demonstrated its strong shale inhibition performance. The rock treated by WBDF containing catechol-chitosan biopolymer had higher tension shear strength and uniaxial compression strength than others, which indicates that it can effectively strengthen the rock and bind loose minerals in micro-pore and micro-fracture of rock samples, owing to the strong adsorption of catechol group on the rock surface and the wrapping effect through hydrogen bonding and Metal chelation. The rheological and filtration property of the WBDF containing catechol-chitosan biopolymer is stable before and after 130°C/16h hot rolling, demonstrating its good compatibility with other WBDF agents.

Abstract ID: 631

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Textiles and Fabrics

Keywords: compression socks, wearing-impacts, tensile decay, areal decay

Assessment of compression socks to different mechanical impacts using cut-strip method

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The aim of this research is to investigate how the performance of compression socks deteriorates due to expected induced wearing mechanical impacts. Wearing mechanical impacts influence the durability parameters i.e. tensile decay and dimensional decay of compression socks. In this study, three unwashed cut-strips were analyzed and compared with hand washed samples for tensile and areal decay. For tensile decay, cut-strip samples were tested for their reaction to a constant rate of loading and unloading, cyclic loading effect at 1st and 15th wearing cycles extended for ± 5 mm and effect of dwell time (3 minutes) at three different extension levels; 25%, 50%, and 75%. Novelty of this research is to relate dynamic performance of compression socks of cut-strip method, using commonly available simple tensile testing machine. For dynamic evaluation, no study, exist in which cut-strips have been evaluated along the both course and wale directions simultaneously. All the results were statistically analyzed.

Abstract ID: 632 / Poster: 15

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Polymeric composites

Keywords: biodegradable polymers, surfactant, composites, eco-friendly wet wipes

Eco-friendly composite materials based on biodegradable polymers and surfactants

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The exponential increase in the use of single-use plastics, including especially wet wipes, in modern society and the inadequate management of the resulting waste have led to their accumulation in the marine and land environment. In spite of appearances, the wet wipes are harmful for the environment. The materials used for production of the wet wipes are fibers, such as cotton and rayon, as well as non-degradable synthetic polymers like polyester, polyethylene and polypropylene. Due to their resistance to degradation, the wet wipes as debris imported into the marine environment have a widespread negative impact on life in the sea, including physiology-level effects and reduced fitness, reproductive failure, changes in community structure, up to direct death after blockage of intestinal tract of organisms or their entanglement. Additionally, the presence of plastics in marine species for human consumption and the high intake of seafood (fish and shellfish) cause concern about the potential effects of plastics on human health [1-5]. The aim of this research was to obtain composite materials based on biodegradable polymers and surfactants that could successfully replace forbidden in the near future wet wipes. Specific properties and structure of composites was achieved by selection of compatible, degradable polymers and appropriate surfactants. The issue of choosing the method of obtaining these materials was also crucial. The results confirmed that a functional prototype of an ecological wet wipe was developed. Such materials are innovation in materials science and could be significant alternative for harmful, non-degradable wet wipes and will be very helpful in protecting the environment.

Abstract ID: 633

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Polymeric composites

Keywords: filler, hydroxylation, low molecular weight natural rubber, nitration, sulphonation, vulcanizate.

The use of modified cocoa shell in low molecular weight natural rubber compounding.

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Natural rubber has some inherent limitations which have contributed to factors militating against its wider usage in some polymeric product but the quest to improve on some of those limitations has led to this research. The natural rubber was first depolymerized with nitrobenzene to obtain low molecular weight natural rubber (LMWNR). Cocoa shell was collected, dried, grinded, and sieved to 75 μ m size. The sieved shells were subjected to different modification vis-a-vis: hydroxylation, nitration and sulphonation. The samples were characterized by determining the moisture content, ash content, loss of ignition and pH for the modified and unmodified cocoa shell samples. Physico-mechanical analysis of the vulcanizates prepared from the LMWNR and modified cocoa shell samples were determined vis-à-vis abrasion resistance, compression set, tensile strength, elongation at break, modulus at various elongations and hardness test. In addition, optical microscopy and UV-visible spectroscopy of the vulcanizates were also carried out. The observed results showed that the vulcanizates from the modified cocoa shell samples were found having better properties in terms of tensile strength and elongations. In fact, sulphonated modified samples were found better than nitrated, which was better than hydroxylated samples. Above all, all the vulcanizates gave properties that will find useful applications in rubber products.

Abstract ID: 634

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Nanostructured materials for advanced batteries

Keywords: Silicon anodes, Graphene, Lithium-ion batteries, Patterning technology.

Interfacial improvement of vertical graphene-coated silicon nanocone anodes for lithium-ion batteries

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Silicon is one of the most promising anode materials for lithium-ion batteries, but the application of silicon anodes is hindered by two major disadvantages of tremendous volume change and continuous solid–electrolyte (SEI) formation. Nanotechnology and graphene coating have been applied to silicon anodes to achieve excellent lithium-ion batteries. However, the exclusive influence of graphene coating on SEI formation is difficult to exhibit distinctly because of morphological irregularity of most nanostructured anodes. Here, the silicon nanocone (SNC) model anode and the coating patterning technology have been combined to demonstrate the significant influences of vertical graphene coating on the electrochemical performance, SEI formation, and structural stability of the silicon anodes. The 3D graphene coating can better accommodate the volume change, facilitate lithium transportation, and promote the electronic conductivity of the SNC electrode. Electrochemical test indicates that the SNC/graphene (SNC-G) electrode has longer cycle life (1715 cycles) and higher Coulombic efficiency (average 98.2%) than the SNC electrode. Moreover, the SNC-G electrode also shows better rate capability and lower electrode polarization. With the patterned electrode, the SNC-G area and the SNC area can be tested under exactly the same condition for making the comparison. As cycle number increases, SEI gradually covers the SNC area while the structure is severely damaged. As a comparison, the SEI on the SNC-G area is much less and the structure retains stable for 100 cycles, which can be attributed to the high electrical conductivity, excellent chemical stability, and remarkable mechanical strength of the vertical graphene coating. The work clearly indicates the improved electrochemical performance, SEI formation, and structural stability attributed to the graphene coating, and the as-proposed patterning technology is of significant guidance for comparative research on coating materials.

Abstract ID: 635

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Applications of low dimensional, nano and 2D materials

Keywords: Comfort, Functional, Nanoparticles, UV protective.

Superhydrophobicity, UV protection and comfort properties of TiO₂ nanoparticles coated cotton fabrics

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The present study is focused on development of multifunctional cotton fabric while having good physiological comfort properties. The functional properties developed include superhydrophobicity (Lotus effect) and UV protection. For this, TiO₂ nanoparticles along with fluorocarbon and organic-inorganic binder have been used to optimize the multifunctional properties.

Deposition of TiO₂ nanoparticles with water repellent finish on cotton fabric has been carried out using pad dry cure method at fix parameters. The morphology and elemental composition of as-deposited particles has been studied by using SEM and EDS. The chemical composition of nanoparticles was determined using energy dispersive spectroscopy. The treated samples exhibited excellent water repellency and UV protection factor. The study of comfort properties of fabric showed that it had excellent physiological comfort properties. Optimized concentration of water repellent chemical (50g/l) was used in formulations with TiO₂ nanoparticles and organic-inorganic binder. 4 formulations were prepared according to design of experiment. The formulations were applied to cotton fabric by roller padding at room temperature (15–20 °C). Surface morphology was investigated via SEM images. EDS analysis was also carried out to analyze composition and atomic percentage of elements. The water contact angle (WCA) of cotton fabric increases with increase in TiO₂ nanoparticles concentration. The water sliding angle (WSA) decreases and gains minimum value at same concentration of TiO₂ at which WCA was highest. It was seen samples treated with formulations of TiO₂ nanoparticles exhibits excellent UPF, UV-A and UV-B blocking. However, there was no significant deterioration of air permeability. The water vapor permeability was also slightly decreased but is acceptable. It can be concluded that there is no significant change in both air and water vapor permeability after nanoparticles coating on the surface of the cotton fabric. The coated cotton fabric has little effect on the stiffness. Stiffness of coated samples was not increased significantly thus comfort of cotton fabric is not decreased. This functionalized cotton fabric also exhibits good physiological comfort properties.

Abstract ID: 636

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Composite structures in civil engineering

Keywords: Composite Section, Cold-formed Steel, Oriented Strand Board, Buckling, I-Section

A Review and Preliminary Study of the Composite Section Incorporated with Cold-formed Steel and Oriented Strand Board

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Cold-formed steel (CFS) is a steel-based material with a variety of shape, grade and thickness which always be used as a structural or non-structural component in building such as roof truss system and wall frame panel. CFS with a lot of advantages such as highest strength-to-weight ratio, lightweight, termite resistance and corrosion resistance is becoming popular. However, CFS with the thin surface is tending to fail in buckling on a short and slender section either as a beam or column. In addition, the CFS section is failed due to local, distortional and global buckling, and web crippling when the load applied. Therefore, a CFS channel section with double intermediate web stiffener is selected as flange element at the top and bottom of the new section. A CFS channel section with web element of 75 mm, flange element of 34 mm, lipped of 8 mm and thickness of 1 mm are chosen. With the intention of solving the buckling problem, CFS is proposed to be a composite section by connecting with oriented strand board (OSB) as a web element using fastener. The composite section is produced into I-section with single or double OSB web element. Hence, CFS Flange OSB Web I-section is proposed as a solid symmetrical section and produced a stable and stiffen section under flexural or compression condition. The main objective is to review the previous study of CFS with other material to produce the composite material and introduce the development, and preliminary study of the new section. There are 9.20% and 5.84% of percentage difference of ultimate load between the CFS single web and double web and without OSB section, respectively. Lastly, the composite section tends to save the production cost, reduce the maintenance cost and influenced to be an innovation section with supporting the Malaysia sustainable development programme.

Abstract ID: 637 / Poster: 29

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Biodetection

Keywords: Surface Plasmon Resonance, biosensor, polarimetry

Adaptable Surface Plasmon Resonance Polarimetry System with variable levels of sensitivity and tunable dynamic ranges

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Surface Plasmon Resonance (SPR) technique has been widely used in sensors due to its unique features, e.g. high sensitivity, real time monitoring, lab-free detection, high-throughput, biological friendliness, etc. The author presents an SPR polarimetry system adopting a custom designed CMOS camera that could deliver a sensitivity up to 1×10^{-7} RIU and a dynamic range of 0.1 RIU. This SPR system could also deliver a variable level of sensitivity within the range of 10^{-6} RIU to 10^{-7} RIU at corresponding dynamic ranges. The unique feature of this system is that a certain combination of sensitivity and its corresponding dynamic range could be shifted to theoretically any refractive indices. As widely accepted, high sensitivity has to compromise with narrower dynamic range, this induces the huge limitation in the SPR biosensor's applications. If both high sensitivity and wide dynamic range are the goals of designing a biosensor, complicated SPR optical systems and usually together with massive data processing are necessary. The author here presents a unique solution to solve this problem by providing an adaptable SPR system, and the only operation is to alter the polarizer and analyzer angles so the response curve could be shifted to the desired refractive index range without any changes in the curve shape, meanwhile, there is no moving parts in this system during binding/sensing process once the polarizer and analyzer angles are fixed. In other words, this system could deliver variable levels of sensitivities within various dynamic ranges, also could deliver 10^{-7} RIU sensitivity at any refractive index or dynamic range as wide as 10^{-1} RIU at any refractive index by shifting the response curves.

Abstract ID: 638

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Large Scale Coating and Industry

Keywords: TBC, HTSPE, Erosion resistance, APS.

**INVESTIGATION OF THERMAL BARRIER COATINGS BOND AND TOP COAT
HIGH TEMPERATURE SOLID PARTICLE EROSION RESISTANCE**

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With the increase of the world population, the need for energy increases. Gas turbines have an important place in the energy sector as well as in the aviation industry. Thermal barrier coatings (TBC) commonly used in gas turbines to protect hot path components in gas turbine are increasingly important. These coatings are exposed to solid particle erosion (SPE) at high temperatures due to their environment and hot combustion gases small particles. Therefore, the resistance of thermal barrier coatings against high temperature solid particle erosion (HTSPE) needs to be studied in detail. In this study, NiCrAlY and NiCoCrAlY metallic powder used bondcoats were deposited on the substrate by Atmospheric Plasma Spray (APS) and yttria (partially) stabilized zirconia (YPSZ) (8 wt.% Y₂O₃ + ZrO₂) was deposited on top coat by APS. High temperature solid particle erosion (HTSPE) tests were performed at room temperature and elevated temperatures. The impingement angles used in the tests were 30°, 60° and 90°, while the impact velocity was 53 m/s. SiO₂ erodent with an average diameter of 250 µm was used. As a result of the experiments, erosion wear resistance of TBC systems formed by bondcoatings coated with different metal powder using the APS method and the adhesion rates of these coatings to the surface were obtained.

Abstract ID: 639

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Multifunctional composites

Keywords: high molecular polymer, high temperature, thermoviscosifying, hydrophobic association

Synthesis and Application of Thermoviscosifying High Molecular Polymer

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Using high molecular polymers as admixtures have always been a hot topic in the oil exploration and development. However, due to the defects of high temperature decomposition failure of traditional high molecular polymers, the applications of high molecular polymers in high temperature drilling and completion are severely limited. To solve the problem, we introduced rigid monomers and hydrophobic monomers onto the traditional AM/AMPS copolymer to synthesize a novel thermoviscosifying high molecular polymer whose viscosity increases upon increasing temperature can match the temperature change in downhole. The high molecular polymer can effectively solve the problems of high temperature decomposition failure of the conventional high molecular polymer admixture and settlement instability caused by high temperature thinning. This new polymer exhibits strong water repellency so that it exists in aqueous solution in the form of particles under low temperatures. Therefore, it has no adverse effect on the viscosity of the aqueous solution under low temperatures. When the temperature increases, the solubility of polymer will increase and the molecular chain will further extend, which induces the thermoviscosifying phenomenon. The infrared spectrum, element analysis and gel chromatography were used to represent and measure the molecular structure and molecular weight of the novel thermoviscosifying high molecular polymer, and the feasibility of using thermoviscosifying high molecular polymer as the drilling fluid plugging agent, fracturing fluid thickener and oil well cement settling stabilizer was discussed in this paper. This study offers a promising solution to greatly enhance the temperature resistance of polymer admixtures and provides suggestive insights for the development of admixtures in the downhole working fluid such as drilling fluids, fracturing fluids and cement slurries.

Abstract ID: 640

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

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

Keywords: Molybdenum selenide, Field-effect transistor, Electronic transportation, Swift heavy ion irradiation, Latent track

Effect of swift heavy ion irradiation induced latent tracks on the electronic transportation behavior in multilayer MoSe₂

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We investigated the electrical properties of MoSe₂ field-effect transistors (FETs) irradiated by swift heavy ions (SHIs) with ion fluences range from 1×10^9 ions/cm² to 6×10^{10} ions/cm². The source-drain current I_{ds} decayed after irradiated with increasing fluences. A reduction of the carrier mobility was observed in the SHI irradiated devices, which would contributed to latent track caused strong localized states in MoSe₂. Latent tracks with amorphous structure in MoSe₂ are confirmed by high-resolution transmission electrical microscope (HRTEM) and atomic force microscope (AFM) images. Electronic transportation mechanism in SHI irradiated MoSe₂ is discussed in detail. This study enriches our understanding of SHI irradiation caused latent tracks in multilayer MoSe₂ and enlightens us to investigate the influence of latent tracks on the electronic transportation in other 2D materials.

Thursday, 22/Aug/2019 3:24pm - 3:36pm

Abstract ID: 641 / FTF-2: 8

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Organic and polymer film

Keywords: super-hydrophobic microtube, flow resistance, surface heat transfer coefficient

Fabrication of Super-Hydrophobic Micro-Tube and Studies on Water Convective Heat Transfer in the Micro-Tube

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Super-hydrophobic/hydrophilic micro aluminum tubes of 0.68mm inner diameter were fabricated with a two step procedure of chemical etching and then surface chemical modification. Firstly, the inner wall of an aluminium micro-tube is treated with 'chemical etching', converting the original hydrophilic inner surface into super-hydrophilic. The water contact angle for the super hydrophilic surface approaches to 0 degree. And then, the super-hydrophilic wall is chemically modified with a kind of polychloroalkelsalane(PAS), forming a thin organic film and further converting the wall into super-hydrophobic. The water contact angle for the super hydrophobic surface is greater than 150 degree. Water drop behaviors on the inner walls of super-hydrophobic and super-hydrophilic micro-tubes are shown in Fig.1. The tiny water drops on the super hydrophobic inner wall appear as spherical balls, whereas, those on the super-hydrophilic inner wall spread and wets the wall.

(a) (b)

Heat transfer and fluid flow of water flowing laminarily in the super-hydrophobic/hydrophilic microtube were studied experimentally. The results show that the air-layer existing in the micro - nano hierarchical structures of the super-hydrophobic surface decreases flow resistance evidently and the heat transfer coefficient decreases a little, which is still higher than the superficial heat transfer coefficient while considering the heat conduction of stationary nanolayer of air. It is supposed that eddy flow is generated in the micro-nano bubbles by the slip flow of water at the tube wall, which enhances the heat transfer. With water flow and heat transfer in the super-hydrophobic micro-tubes investigated, hemisphere heat transfer model for caves on the super-hydrophobic surface is presented. The control equations in spherical coordinates are selected and the model is numerically simulated with FLUENT. The simulate results agree with experiment results well. Air existing in the coarse structure on the super-hydrophobic surface forms eddies due to existence of slip velocity on the wall of the tube and it can enhance heat transfer in the tube.

Abstract ID: 642

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Plenary

Topics: Clinical trials

Keywords: Biomaterial, CAD-CAM technology, 3D-printing, Laser-sintering, Titanium meshes, cross-linked collagen membrane.

Three-dimensional Guided Bone Regeneration (GBR): Customized Titanium laser-sintered meshes with and without collagen membranes.

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Background: The presence of alveolar ridge deficiencies is considered a major limitation to achieve an implant-prosthetic restoration with high aesthetics and stability over time. Guided Bone Regeneration (GBR) can be considered an effective solution for bone augmentation. The most advanced technology of GBR is the customized titanium mesh, which is developed with a fully digital work flow system. The aim of this study is to evaluate complications and bone augmentation rates after GBR, based on customized meshes with or without collagen membranes. Materials&Methods: After ethical committee approval of University of Bologna (Italy), 30 patients with bone defects were enrolled and treated according to the study protocol. During reconstructive surgery (T0), patients were randomly divided into two study groups: 15 patients were treated by means of a custom-made mesh without collagen membrane (Control Group), while 15 patients were treated by means of a custom-made titanium mesh with a collagen membrane (Test Group). After 6 months (T1), re-entry surgery was completed to remove the meshes, evaluate the augmented volume and to place implants in the augmented sites. After 3 months (T2), soft tissue management was accomplished with implant exposure and a connective tissue graft, before prosthetic restoration (T3). A statistical analysis of recorded data was performed to investigate any statistically significant differences between the study group and statistical significance was set at $\alpha=0.05$. Results: Up to date, all patients underwent to GBR surgery using customized titanium meshes: 26 out 30 patients underwent to re-opening surgery and implant surgery and they were considered for statistical analysis. Two early exposures and two late exposure of the meshes were observed in the control group (28.6%); one abscess without exposure and one early exposure were noted in test group (16.7%). Mean values of PBV and RBV in the control group were 1.11cc and 0.85cc; while, in the test group, 1.25cc and 1.09cc, respectively. As consequence, the regeneration rates in both study groups were 76.6% and 87.2%, giving a significant statistical difference ($P=0.046$). Pseudo-periosteum type and bone density were not statistically different over the 2 groups ($P=0.67$). Crestal bone loss of restored implants appeared stable and less than 1.5mm in both groups ($P<0.001$), resulting in success rates of 100%. Finally, statistical analysis revealed significant differences in bone density between the mandible and maxilla ($P=0.03$). Conclusions: The preliminary results of this randomized clinical trial showed that GBR using customized mesh is a reliable and predictable solution for bone augmentation. Both approaches result in interesting outcomes in vertical and horizontal defects. Complication and regeneration rates seem to be better in group with mesh and collagen membrane compared to mesh alone.

Abstract ID: 643

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Biomaterial surfaces

Keywords: plasma immersion ion implantation; Zn/Ag co-implantation; biological properties; antibacterial properties.

Effects of Zn and Ag ratio on cell adhesion and antibacterial properties of Zn/Ag co implanted TiN coatings

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Titanium and its alloys have good biocompatibility and mechanical properties, but they do not possess antibacterial properties and have biological inertia, which restricts the repair of hard tissue. In this study, titanium nitride (TiN) was deposited on the surface of titanium alloy to enhance its hardness and corrosion resistance, then Zn and Ag were co-implanted by plasma immersion ion implantation (PIII), and different implantation ratios (Zn:Ag=1:1; 2:1; 3:1) were set up to investigate the effects of Zn and Ag ratio on cell adhesion and antibacterial properties. In this study, the electrochemical workstation was conducted to test the corrosion resistance of samples under physiological conditions. Contact angle measurement and protein adsorption experiments were used to explore the relationship between hydrophobicity, protein adsorption, cell spreading and proliferation. The proliferation of cells on the surface of samples was analyzed by the MTT assay and the morphology of cells was observed by SEM. The bacteria colony of each sample was counted to measure antibacterial properties. The results demonstrated that the cell adhesion and antibacterial properties were improved at different implantation ratios compared with the control group(TiN). With the increase of Zn implantation ratio, the proliferation of cells on the surface of the samples was more obvious, the morphology of cells was more plump, and the junction between cells was closer, which as shown in Fig.1. Meanwhile, the samples had good antibacterial properties.

Abstract ID: 644

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Applications of low dimensional, nano and 2D materials

Keywords: Gold nanoparticles; soursop; breast cancer; contrast agent; pharmacokinetics; photothermal therapy

In Vivo Contrast Studies on Breast Cancer tumor in Sprague dawley rats and Photothermal Therapy Using Gold Nanoparticles

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Gold nanoparticles are synthesized and stabilized using Soursop fruit extract in a greener way. The nanoparticles are characterized using various techniques like UV-Vis spectroscopy, Transmission Electron Microscopy, Zeta potentiometer and Fourier Transform Infrared Spectroscopy. The particles are easily soluble in water, stable for more than six months and viable to breast cancer cell lines MCF-7. This study demonstrated the feasibility of gold nanoparticle based molecular cancer imaging, pharmacokinetics studies and photothermal therapy. It was shown that the molecularly targeted tumor is high contrast than the corresponding untargeted tumor. Further, the gold nanoparticles are maximally accumulated in tumor cells. The laser irradiated gold nanoparticles in the tumor site caused irreversible tumor tissue damage without destroying the healthy cells. All the rats treated with gold nanoparticles and Laser are survived even after five months with no evidence of tumor recurrence.

Abstract ID: 645

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Structural, Electronic, Optical and Magnetic Properties

Keywords: GFET, electrical characteristics, swift heavy ions, irradiation effects, optimization

Graphene electrical properties modulated by swift heavy ion irradiation

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Changes in electrical properties of graphene devices induced by energetic ion irradiation are very important for their application in harsh radiation environment. We investigate the modulating behavior of electrical properties of graphene-based device irradiated by swift heavy ions (SHIs). Graphene field effect transistors (GFETs) were irradiated by 1.79 GeV Ta ions and it was found that at lower fluence (10^9 ions/cm²~ 10^{10} ions/cm²), the SHIs irradiation can effectively optimize the performance of GFET while at higher fluence, the electrical properties of the devices were significantly deteriorated after the irradiation process. The length and width ratio of the graphene ribbon, electronic energy loss (dE/dx)_e of the SHIs and the irradiation fluence are the three factors that determine the improvement in performance of the GFET. In this work, Raman spectroscopy was employed to figure out the correlation between the changes in electrical performance of GFET and initial defect density in graphene. The competition among various factors such as the doping, local annealing and defect creation dominates the GFET performance. Moreover, not only the defects and doping in graphene make significant contribution to the deterioration of electrical properties of GFET but also the defects in substrate and doping at SiO₂/Si interface can contribute substantially to these changes. The resistance, carrier mobility and position of Dirac point can be modified by the SHIs irradiation, which paves a way for the optimization of GFETs. This work provides an important reference for the graphene based irradiated devices in aerospace electronics as well.

Abstract ID: 646

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Structural, electrical, mechanical and optical of low dimensional, nano and 2D-layered oxides, nitrides and sulfides

Keywords: magnetron sputtering; TiB₂/BN multilayer; thermal stability; heating rate.

Influence of temperature rise rates on the interfacial structure and mechanical stability of TiB₂/BN superlattice coatings

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The multilayered modulation structure and mechanical properties of TiB₂/BN superlattice coatings deposited on monocrystalline silicon by magnetron sputtering were investigated using extensive measurements. The influences of temperature rise rates on microstructure and mechanical properties of annealed TiB₂/BN multilayers were discussed. The nanoscale TiB₂/BN multilayers were annealed in vacuum at 700°C for 10, 30, 60 and 120 min. The thermal stability and oxidation resistance of TiB₂/BN multilayers was examined by second annealing performed in annealing furnace at different heating rates in air. The results showed that different crystallization orientations developed in BN interlayers during the annealing process. The good thermal stability in properties of TiB₂/BN superlattice coatings should be related to the favorable thermal stability of BN interlayers and superlattice structure. The annealing process led to a significantly enhancement in hardness, adhesion strength, as well the friction coefficient. The high oxidation resistance of the films was attributed to the presence of BN layer interface that acted as a barrier to O diffusion. The BN (002) and c-BN (111) textures were kept after 30 min annealing time, also giving a significant contribution to stable hardness.

Abstract ID: 647

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Biocomposites

Keywords: Biocomposites, Lignocellulosic, Insulator, Thermal conductivity, Dielectrical

Mechanical, Thermal and Dielectric Properties of Poly Propylene Blended with Lignocellulosic for Insulating Biocomposites Material

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In this experimental study, the possibilities and potential of the polymer and lignocellulosic material for insulation biocomposites are studied. Element analysis was used to characterize the polypropylene (PP) and kenaf core fiber (KCF) in the biocomposites material. Combination of polymer and natural fibre were blended in internal mixer at 150°C for 15 minute. Compounding were compressed then the sheets of KCF board composites were determined for flexural properties, i.e. flexural strength and flexural modulus as mechanical properties, thermal conductivity and dielectrical properties. The flexural properties were found to be on a reasonable level. Thermal conductivity of KCF composites showed a good potential for insulating material composites. KCF board showed a value of 0.0823 compared to the others composites like cotton. In this study, dielectrical properties of the composites achieved the standards for insulator biocomposites. In conclusion, the combination of polymer and lignocellulosic showed huge potential for insulation biocomposites materials in terms of thermal conductivity and dielectrical properties.

Abstract ID: 648

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Biocomposites

Keywords: Citric acid, termite resistance, fungus resistance, physical, mechanical

Physico-mechanical and biological properties of citric acid bonded rubberwood particleboard

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Citric acid was used in the current study to replace the urea formaldehyde (UF) as binding agent due to its good adhesivity for wood. Citric acid is an organic polycarboxylic acid containing three carboxyl groups and was used as cross-linking agent to enhance the properties of wood. Rubberwood particles with 3% moisture content were obtained from a local plant. Citric acid in powder form were diluted into distilled water to attain 60% solid content. The dosages of citric acid used was 10%, 15% and 20% based on the oven dried weight of the rubberwood particles. The citric acid solution was mixed with rubberwood particles in a blender and was then formed into a mat before hot pressing. The formed mat was pressed at temperature of 180 °C for 7 min. Particleboard with 680 kg/m³ and dimensions of 340 mm x 340 mm x 12 mm were produced. A set of particleboards made from 10% UF resin were served as control. Properties such as thickness swelling (TS), water absorption (WA), bending strength, resistance against termites and white rot fungus were evaluated. The results revealed that both TS and WA of the citric acid were higher than that of the UF-bonded particleboard. However, as the dosage of the citric acid increased to 20%, the TS and WA were improved. Significantly inferior bending strength were observed in the citric acid bonded particleboard. Nevertheless, citric acid bonded particleboard displayed better biological resistance against termites and fungus compared to UF-bonded particleboard. Another advantage of citric acid bonded particleboard is they resulted in zero emission of formaldehyde.

Abstract ID: 649**Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)****Invited Talk**

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

Keywords: Conducting polyaniline, Ink-jet printing, Flexible electronics

Successful Journey of Conducting Polyaniline from Non Soluble and Non Process able Powder to Process able, Aqueous, Ink-jet Printable Ink for Flexible Electronics Applications**Milind Vyankatesh Kulkarni**

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Abstract

Among organic conducting polymers, polyaniline (Pani) is regarded as one of the most technologically promising electrically conductive polymers due to its ease of synthesis, low cost, versatile processability and relatively stable electrical conductivity. However, a major problem related to its successful utilization lies in its poor mechanical properties and processability due to its insoluble nature in common organic solvents. In the past few years, much progress has been made to improve both these aspects. Among these areas of progress the approach of the chemical synthesis method and use of functional dopant is more attractive as it eliminates the use of volatile dopant. The functional dopants are introduced in the polymer matrix either by a secondary doping method or by blending the polymer with doping species. We have successfully developed an in situ chemical polymerization process, which yields a processable polyaniline directly without the need for a post-doping process. The reaction is unique, since it is a single step process for the direct synthesis of conducting emeraldine salt phase of the polyaniline and eliminates the post-processing steps which involve: (i) neutralization of the emeraldine salt to form emeraldine base and (ii) reprotonating the base with a second protonic acid.

(a) (b)

Fig.1 Free flowing powder of polyaniline emeraldine salt and pressed pellets using hydraulic press (a) & Polyaniline based ink and inkjet-printed IDT pattern on flexible untreated polymer substrate (b)

Here, we have investigated the processable, aqueous, sulphonic acids doped ink-jet printable polyaniline based ink and successive printing of interdigitated (IDT) pattern on flexible, untreated polymeric substrates and its use as a thin, inkjet printed flexible, humidity sensor. For chemical sensing applications, the more 'open' morphology of inkjet printer films (i.e. a series of connected droplets) may allow rapid diffusion of the water vapour molecules into and out of the film, leading to fast response and recovery times. The advantage of using inkjet print technology for this type of humidity sensor is the high speed and low cost of fabrication as well as the possibility of printing onto flexible substrates. This conducting polyaniline based aqueous ink will also have potential applications in low cost RFID tags, flexible polymer photovoltaic cells and in printed flexible electronics devices. Recently, we have also developed Silver and Gold nanoparticles, Carbon nanotubes (CNTs) and Graphene based ink for flexible electronics devices.

Abstract ID: 650

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Theoretical/Modelling/Computer Simulations Of Functional Materials

Keywords: Semiconductor Nanocrystals, Electrical Conductivity, Localization Length, Blinking Metal Phase

Deciphering the Route to Blinking Metal phase of electrical conductivity in touching semiconductor nanocrystals.

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The present study focuses on modulating the behaviour of electrical conductivity in a system of array of touching semiconductor nanocrystals (NCs) which depends on localization length of the electrons. Such systems show a metal insulator transition (MIT) at a critical carrier concentration n_c . We show that, for a particular parameter regime, even below n_c , the system can exhibit a “blinking metallic” (BM) phase in which it oscillates between insulating phase and metallic phase as the concentration is increased. The BM phase is atypical and an in-depth understanding of parameters governing localization length is required which can pave the way to achieve the BM phase in these systems. The localization length depends on the ratio of energy difference and the tunnelling matrix element $t(n)$ between the states of the neighbouring NCs. This ratio can be tuned by extent of disorder present in the system, the source of which can be either size distribution of NCs or non uniform doping of NCs. This allows us to predict the parameters to achieve the BM phase of electrical conductivity for such systems. We exemplify our results on system of array of PbTe NCs.

Wednesday, 21/Aug/2019 4:51pm - 5:03pm

Abstract ID: 651 / FC: 5

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Photocatalysis

Keywords: Photocatalysis, Hydrogen, Core-Shell, Photonic structure

Photocatalyst designed in core-shell or three-dimensional nanostructure for enhanced photon-to-conversion efficiency for Hydrogen production

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As well as direct energy conversion in solar cells, sunlight can be used as the energy source for water depollution or hydrogen production. These two are inexorably linked as both use photocatalysis as their energy conversion mechanism. Photocatalytic depollution of water has attracted great attention and many studies have been published in the last decade; however, improving photocatalytic efficiency, as well as making the process industrially viable remain challenges. Additionally, the conversion of water to hydrogen fuel using photocatalysis is one of the most promising strategies for industrial-scale production.

Titanium dioxide is by far the most popular photocatalyst; it is cheap, inert and reasonably active. However, TiO₂ has a large band gap (3.2 eV for anatase and 3.0 eV for rutile) can only be excited by UV light, which lower the solar energy conversion efficiency and limit its use in the visible range (small absorbance factor). Therefore, engineering the architecture of the plasmonic photocatalyst in core-shell or 3D photonic crystals leads to the enhancement of light harvesting properties and improved photon-to-energy conversion for hydrogen production. In core-shell nanostructure, the photocatalyst behave as a photonic “NanoLens” mimicking the focusing of light observed for the lens-like epidermal cells [1]. Thus, the core-shell nanostructure acts as a convex nanolens to reinforce the electromagnetic field at the nanostructure surface. Designed in photonic film with chiral nematic structure the mesoporous structure with a 3D architecture, titanium dioxide showed improved efficiency of the conversion of light to energy [2].

The material was characterized by means of different techniques, such as BET, WAXS, polarized optical microscopy, UV-Visible spectroscopy, TEM and Time Resolved Microwave Conductivity (TRMC). TRMC results show an improvement of the charge carrier density produced under illumination at the photocatalyst surface. This strategy enables to avoid the use of higher amount of Nobel metal to reach higher efficiency of photocatalytic production of hydrogen.

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Abstract ID: 652

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Invited Talk

Topics: Anti-cancer therapy

Keywords: Magnetic hyperthermia

Nickel-Zinc Ferrite Nanoparticles: A Potential Heat Generating Material for Magnetic Hyperthermia

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CTAB (cetyltrimethylammonium bromide)-coated $\text{Ni}_x\text{Zn}_{1-x}\text{Fe}_2\text{O}_4$ (x:0.0(1z),0.25(2z),0.5(3z),0.75(4z)) nanoparticles of crystallite sizes 6-15 nm with various stoichiometric ratios were successfully synthesized using co-precipitation technique. The synergistic influences of CTAB coating and Ni^{2+} ions is observed with the increasing saturation magnetization (29 emu/g \rightarrow 49 emu/g) and reduced effective anisotropy constant (K_{eff}) of the nanoparticles. Induction heating study shows the intimate association between the K_{eff} , saturation magnetization and heat dissipation rate of the nanoparticles. $\text{Ni}_{0.75}\text{Zn}_{0.25}\text{Fe}_2\text{O}_4$ nanoparticles of 49 emu/g ascend to a specific absorption rate of 347 W/g at the minimal concentration of 2 mg/ml within a very short time-period of 1.5 mins evincing the effective relaxation mechanisms at the applied field and frequency. This study presents a potential heat generating material for the application of magnetic hyperthermia.

Abstract ID: 653

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Composite structures in civil engineering

Keywords: arbon fiber reinforced polymer, concrete column, initial defect, critical defect size, finite element analysis

The effect of defect size on the integrity of CFRP-confined concrete column

许颖

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This paper explores the effect of defect size on the integrity of CFRP (Carbon Fiber Reinforced Polymer)-confined concrete, which governs the strength and deformability of the structural element. Qualitative theoretical analysis and experimental investigation are carried out and compared to investigate the mechanical behavior and failure mode of CFRP confined concrete column with initial defects under axial and eccentric compression. The variation of criticality defect is investigated by varying the layer number of CFRP and cross-section size of concrete columns. The results demonstrated that for a CFRP-confined concrete column, the propagation of the initial defect may not lead to global failure. In general, such a phenomenon alters the confining pressure provided by the FRP, leading to stress redistribution and weakening of the structure. Deformation behavior and final failure greatly depend on the initial defect size.

Abstract ID: 654

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

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

Keywords: NaNbO₃, hydrogen generation, type-II heterojunction, charge carriers, hybrid density functional theory calculation

Tuning the electronic structures, work functions, optical property and stability of bifunctional hybrid graphene oxide/V-doped NaNbO₃ type-II heterostructures: a promising photocatalyst for H₂ production

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The depleting sources of non-renewable fossil fuels and their adverse effect on the environment have driven the global interest to find an efficient and suitable material for hydrogen generation via a water splitting process. Although NaNbO₃ has several vital properties as an efficient photocatalyst, its wide band gap energy reduces its photocatalytic performance only to the ultraviolet region. In this theoretical study, a bifunctional graphene oxide (GO)/V-doped NaNbO₃ (100) heterostructure photocatalyst having a high stability and activity is studied for the first time using a hybrid density functional theory calculation with a dispersion correction. The band edge potentials, work functions, thermodynamic stability, optical property (absorption coefficient) and electronic properties (density of state, band structures and charge carrier mobility) are also considered in this study. During this process, NaNbO₃ is doped with V⁵⁺, which is then coupled with a GO sheet. The suitable type-II heterojunction structure between NaNbO₃ (100) and GO sheet promote the interfacial charge migration to restrain their recombination rate, thereby improving the activity of hydrogen generation. Moreover, the coupled GO sheet can offer conductive electron channels for the separation of electrons, and hence further improve the photoresponse of NaNbO₃. The GO/V-doped NaNbO₃ (100) heterostructure is a direct band gap semiconductor with a smaller effective mass compare with the pure NaNbO₃, which shows that the heterostructure has a higher charge carrier mobility. Thus, the resulting bifunctional GO/V-doped NaNbO₃ (100) heterostructure is endowed with a suitable band alignment, narrow band gap, negatively charged O atoms on the NaNbO₃ (100) surface and enhanced separation of charge carriers. The findings in this study are intended to offer new and valuable insights into the design of GO-based photocatalyst with visible light activity.

Abstract ID: 655 / Poster: 16

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

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

Keywords: SrTiO₃; environmental and energy crises; type-II band alignment; environmental contamination; hybrid DFT

First-Principles Study of Cubic SrTiO₃ with Perovskite-Type Materials MTaO₃ (M = Na, K) for Environmental Remediation

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Due to increasingly global environmental and energy crises, visible light semiconductor photocatalyst with a tuneable bandgap and optical properties have received attention. This study aid in the design of bifunctional MTaO₃/SrTiO₃(010) (M = Na, K) heterostructures photocatalyst material for environmental remediation. In this study, the stability, electronic and optical properties of coupled MTaO₃ and SrTiO₃ were systematically studied using the hybrid HSE06 method. The MTaO₃/SrTiO₃(010) heterostructures show high photocatalytic activity under visible light irradiation with good stability and reduced bandgap compared to the bulk SrTiO₃. The heterostructures formed a type-II band alignment to accelerate the interfacial charge transfer process and the photocatalytic activity. By comparing the relative ratio of effective mass, we could conclude that MTaO₃/SrTiO₃(010) heterostructures has not only superior mobility of charge carriers, but also higher separation of photoinduced electrons and holes. The band alignment results showed that the MTaO₃/SrTiO₃(010) heterostructures were highly efficient for pollutants degradation and energy conversion. Significantly, the origin of the enhanced photocatalytic activity was observed from the O 2p state of SrTiO₃ to the Ta 5d state of MTaO₃. In summary, this study shows a key role of SrTiO₃ as an electron donor to enhance the optical properties and stability of MTaO₃/SrTiO₃(010) heterostructures.

Abstract ID: 656

Symposium 5: Functional 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, SERS, lab-on-a-chip, stimuli-responsive, origami

Self-folding hybrid graphene skin for 3D biosensing

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Biological samples such as cells have complex three-dimensional (3D) spatio-molecular profiles and often feature soft and irregular surfaces. Conventional biosensors are based largely on 2D and rigid substrates, which have limited contact area with the entirety of the surface of biological samples making it challenging to obtain 3D spatially resolved spectroscopic information, especially in a label-free manner. Here, we report an ultrathin, flexible skin-like biosensing platform that is capable of conformally wrapping a soft or irregularly shaped 3D biological sample such as a cancer cell or a pollen grain, and therefore enables 3D label-free spatially resolved molecular spectroscopy via surface-enhanced Raman spectroscopy (SERS). Our platform features an ultrathin thermally responsive poly(N-isopropylacrylamide)-graphene-nanoparticle hybrid skin that can be triggered to self-fold and wrap around 3D micro-objects in a conformal manner due to its superior flexibility. We highlight the utility of this 3D biosensing platform by spatially mapping the 3D molecular signatures of a variety of microparticles including silica microspheres, spiky pollen grains, and human breast cancer cells.

Abstract ID: 657

Symposium 6: Functional Thin Films (FTF)

Keynote

Topics: Thin Films in Photovoltaic Cells and Energy

Keywords: thin film, circular economics, solution to climate change, solar powered cars

Thin Solar Film --- ALL Solar Powered Cars

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Taking several areas in technology, science and energy that link together in order to be less expensive, reduce and reverse climate change which are available today. Case in point are the all solar powered cars that come from a company in China which produces thin film solar which were designed and used for buildings but now also as the only power for cars and buses. The vehicle solar panels are then able to be reused in the future for solar power in homes, businesses, governments, parks, communities and other areas. This process is a new way to do economics and is Circular Economics which has been implemented in the EU and beginning in China.

Solar energy is utilized as the main driving force, which overturns the charging mode of traditional electric driving and fixed charging facilities. Meanwhile, it can also make the vehicles directly utilize solar energy like chlorophyll, which satisfies travel demand and will not generate any pollution at the same time. Besides, at the news conference, you will witness the world's first drivable wholly solar-powered car. The modules of thin-film solar are perfectly integrated into the roof and body of the vehicles, providing clean energy for vehicles through the sunniness, which greatly enhances environment protection and driving comfort of vehicles

Wednesday, 21/Aug/2019 5:00pm - 5:12pm

Abstract ID: 658 / FBB: 6

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Computational studies of Biomaterials

Keywords: Laser irradiation; Human breast; Tumor; Skin tissue; Power density

Thermal Influence of Laser Irradiation on Human Breast with Tumor

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In this paper, a thermal model of a human breast with a tumor was developed as a multi-layer medium; skin, fat, and tumor. In this model, we will take into account the internal heat source generated within the human breast from the chemical reactions of the tissue and the lag-time to study the response time of the tissue takes due to the perturbation in the context of non-Fourier's heat conduction with one relaxation time. The materials parameters of the human breast and the tumor have been used. Laplace transforms have been applied, and the inversions have been calculated numerically. We studied the thermal loading due to laser irradiation through the human breast with different values of time, depth, relaxation time, and power density. The thermal damage quantity has been calculated to the three layers by using the Arrhenius burn integration approach. It was shown that all that parameters have significant effects on the human breast with the tumor. This work will help improve the use of laser in the treatment of breast tumor.

Abstract ID: 659

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Anodes and cathodes Materials

Keywords: Graphene, Single-Atom Catalyst, Sulphur Cathode, High Mass-Loading, Energy Storage.

Cobalt in Nitrogen-Doped Graphene as Single-Atom Catalyst for High-Sulphur Content Lithium-Sulphur Batteries

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Lithium–sulphur (Li–S) battery has attracted a great deal of attention for next-generation energy storage for its high theoretical capacity, however, three quarters of the Li–S battery’s theoretical capacity comes from the slow liquid–solid phase transformation of soluble Li_2S_4 to solid Li_2S . And the sluggish kinetics of this process leads to an accumulation of soluble Li polysulfides (LiPSs) in the cathode area, from which, their inevitable diffusion to anode results in “shuttle effect”, and their arbitrary precipitation of solid Li_2S on the cathode surface results in large Li_2S particles that are difficult to be reused. Such detrimental effects are more pronounced at the increased S mass ratio in cathode, thus limiting the practical gravimetric capacity per mass of the cathode.

Single-atom catalysts (SACs) are monodisperse single atoms supported on solid substrates with a theoretical 100% atom utilization efficiency and combine the advantages of both heterogeneous and homogeneous catalysts. Moreover, a well-defined active centre made from a single-atom can be used as a model system to acquire in-depth understanding of the catalytic reaction pathway.

Here, we propose a SAC comprising Co atoms embedded in a nitrogen-doped graphene framework (Co-N/G) as a cathode for Li-S batteries. The coordination configuration of Co single atoms at the atomic level, were identified by high-angle annular dark field imaging and extended X-ray absorption fine structure. A precise description of the atomistic structure of Co-N/G allowed us to combine operando X-ray absorption spectroscopy and first-principles calculation to identify that Co-N-C moieties facilitate both the formation and decomposition of solid Li_2S in discharge and charge processes, respectively. Consequently, the S@Co-N/G composite, with a high S mass ratio of 90 wt.% in the composite and S loading of 6.0 mg cm^{-2} on the electrode disk, exhibits an areal capacity of 5.1 mAh cm^{-2} with capacity fading rate of 0.029% per cycle over 100 cycles at 0.2 C. Our study revealed the catalytic effects of the isolated Co-N-C moieties on the electrochemical reactions of LiPSs, which points out new strategies to design sulphur cathodes that can effectively mitigate the tradeoff between the sulphur mass loading and electrochemical reaction kinetics.

Key Words: Graphene, Single-Atom Catalyst, Sulphur Cathode, High Mass-Loading, Energy Storage.

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Abstract ID: 660

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: RGO-Au Nanocomposites, SERS, Photoluminescence, Biosensor, Photocatalysis

Multifunctional Reduced Graphene Oxide (RGO) Wrapped Circular Au Nanoplatelets: Enhanced Photoluminescence, Surface Enhanced Raman Scattering, Photocatalytic Water Splitting and Non-enzymatic Biosensors

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In the recent past, multifunctional nanocomposites have attracted considerable attention owing to their large scale prospective applications.¹⁻⁵ Herein, we demonstrate the synthesis, characterization and multifunctional properties of RGO wrapped Au nanoplatelets. We have characterized the sample by FESEM, HRTEM, EDS, STEM-HAADF, EELS, XPS studies. It has been shown that the RGO wraps a large number of 2D circular Au nanoplatelets (diameter ~ 15 nm). A large enhancement in intensity of Raman spectra was observed due to the surface-enhanced Raman scattering (SERS) resulting from the Au nanoplatelets. SERS enhancement factor (taking 1×10^{-6} M R6G) of GO, RGO and RGO-Au are 7.09×10^{10} , 4.81×10^{10} and 1.01×10^{11} , respectively, at 1375 cm^{-1} while SERS enhancement factor of GO, RGO and RGO-Au are 3.91×10^{10} , 2.25×10^{10} and 1.43×10^{11} respectively at 1632 cm^{-1} . Upon visible light irradiation, the sample exhibits photocatalytic water splitting effect, where photodetection properties of RGO-Au sample is greatly enhanced compared to bare GO by incorporation of Au nanoplatelets.¹ The sample displays excellent non-enzymatic hydrogen peroxides (H_2O_2) and ascorbic acid (AA) sensing property. The value of sensitivity for H_2O_2 is $280.28 \mu\text{A mM}^{-1}\text{cm}^{-2}$ in the linear range of $1 \mu\text{M}$ to 0.8 mM and that for AA is $314.07 \mu\text{A mM}^{-1}\text{cm}^{-2}$ in the linear range of for $25 \mu\text{M}$ to $300 \mu\text{M}$. So, the sample can be used for multifunctional applications in SERS as a substrate, photocatalytic water splitting, photodetectors, and non-enzymatic biosensing.

Key Words: RGO-Au, Nano, SERS, Photoluminescence, Biosensor, Photocatalysis

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Abstract ID: 661

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Electrochemical Supercapacitors

Keywords: Fe₃O₄-RGO Nanocomposite, Fe²⁺/Fe³⁺, Enhanced Magnetism, Energy Storage

Magnetization Enhancement of Fe₃O₄ nanoparticles by attaching onto Graphene Oxide and its Application towards Magnetic Field Dependent Enhanced Electrochemical Energy Storage Performances: An Interfacial Effect

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Here, we have reported about the enhancement of magnetization and blocking temperature of Fe₃O₄-reduced graphene oxide (RGO) nanocomposite, which is formed by embedding Fe₃O₄ nanoparticles onto RGO sheets. We have utilized powder XRD, FESEM, HRTEM, EELS, EDS, FTIR, Raman and XPS techniques to investigate the crystallinity, morphology, phase, composition, purity, and evolution of oxidation states of nanosized Fe₃O₄ (S1) and Fe₃O₄-RGO nanocomposite (S2). EELS, Raman and XPS all together indicate that graphene oxide (GO) has been converted into reduced graphene oxide (RGO) during formation of Fe₃O₄-RGO nanocomposite. Analysis of Fe 2p_{3/2}, Fe 2p_{1/2} peaks in the XPS spectrum of S1 and S2 reveals that Fe²⁺ ions have been converted to Fe³⁺ ions during formation of Fe₃O₄-RGO nanocomposite, which has been proposed as the main reason for enhancement in magnetization. Enhancement of blocking temperature of S2 with respect to S1 is due to the enhancement in size of the magnetic domain in S2. Moreover, we have also studied how the magnetic field enhances the electrochemical energy storage capacity of S2. In the presence of an external magnetic field, the Fe₃O₄-RGO supercapacitor electrode shows enhanced capacitance of 868.89 F g⁻¹ (1.93 times greater), versus 450.61 F g⁻¹ in the absence of any magnetic field, at 5 mV s⁻¹ scan rate. In addition, the energy density and power density of the composite electrode in the presence of magnetic field are noticeably improved to 120.679 Wh/kg and 1.45 kW/kg respectively. This finding suggests the potential revolution of traditional supercapacitors in presence of external magnetic field to improve the capacitance significantly without material replacement.

Key Words: Fe₃O₄-RGO Nanocomposite, Fe²⁺/Fe³⁺, Enhanced Magnetism, Energy Storage.

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Abstract ID: 662

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Electrochemical Supercapacitors

Keywords: Thiospinels, Photocathode, Dye Sensitized Solar Cells, Hydrogen Evolution Reaction, Energy Storage

Fabrication of bimetallic chalcogenides with ease for better performance of DSSCs, hydrogen evolution reaction and as hybrid energy storage material

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Energy is the most fundamental and great challenge in the fast growing era in terms of harvest and storages. Meanwhile environmental issues are major setback in energy production by fossil fuel. Desperately, researchers are looking forward to various smart materials performing multitask from harvesting to storage.1-2 The transition metal based composites especially Mn, Fe, Ni, Co, and Ru made huge impact in various electrochemical applications. In the present scenario, Ni composites are established as high efficiency materials for effective electrocatalyst in HER, OER and also as counter electrode for the DSSCs. Nickel tin sulfide thiospinel composited MWCNTs (M–NiSn₂S₄) are synthesized and fabricated with ease. The metallic conductivity and electrocatalytic activities have played a prominent diverse roles in the (1) design of a counter electrode for DSSCs with 4.67 % efficiency when compared to Pt (5.23 %) at fluorine doped indium tin oxide, (2) development of an efficient catalyst for hydrogen evolving reaction which is similar to Pt with good cyclic stability, exhibits low over potential of -41 mV at the cathode current density 10 mA cm² and Tafel slope of 43 mV/dec using Ni mesh electrode and (3) fabrication of an impressive capacitance materials at graphite sheet electrode will be an alternate to the existing high expensive current collectors like Ni foam with the specific capacitance of 1,200 Fg⁻¹ at current density 1 Ag⁻¹ and long life span such as 92.6 % retained up to 15,000 cycles. As a result, M-NiSn₂S₄ nanocomposite loaded graphite sheet electrode retained high charge density of 96.59 WhKg⁻¹ when power density is 1 WKg⁻¹. Accordingly, a symmetric capacitor has been successfully constructed and studied the performance in the continuous LED glow in two electrode system separated by solid electrolytic film separator made of PVA/KOH (95:5) wt % with good conductivity.

Key Words: Thiospinels, Photocathode, Hydrogen Evolution Reaction, Energy Storage

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Abstract ID: 663

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Photonic and optoelectronic device applications of low dimensional, nano and 2D materials

Keywords: Sn doping in Tellurium Telluride nano-materials, electron holes competition, Seebeck co-efficient, effects of Sn doping on Electrical conductivity, effects on Power factor

Designing and Fabrication of efficient nano-materials for thermoelectric generator

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The electrical and thermal properties of the doped Tellurium Telluride (Tl₁₀Te₆) chalcogenide nano-particles are mainly characterized by a competition between metallic (hole doped concentration) and semi-conducting state. We have studied the effects of Sn doping on the electrical and thermoelectric properties of Tl_{10-x}Sn_xTe₆ ($1.00 \leq x \leq 2.00$), nano-particles, prepared by solid state reactions in sealed silica tubes and ball milling method. Structurally, all these compounds were found to be phase pure as confirmed by the x-rays diffractometry (XRD) and energy dispersive X-ray spectroscopy (EDS) analysis. Additionally crystal structure data were used to model the data and support the findings. The particles size was calculated from the XRD data by Scherrer's formula. The EDS was used for an elemental analysis of the sample and declares the percentage of elements present in the system. The thermo-power or Seebeck co-efficient (S) was measured for all these compounds which show that S increases with increasing temperature from 295 to 550 K. The Seebeck coefficient is positive for the whole temperature range, showing p-type semiconductor characteristics. The electrical conductivity was investigated by four probe resistivity techniques revealed that the electrical conductivity decreases with increasing temperature, and also simultaneously with increasing Sn concentration. While for Seebeck coefficient the trend is opposite which is increases with increasing temperature. These increasing behavior of Seebeck coefficient leads to high power factor which are increases with increasing temperature and Sn concentration except For Tl₈Sn₂Te₆ because of lowest electrical conductivity but its power factor increases well with increasing temperature.

Abstract ID: 664

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Interfaces and interphases

Keywords: Nanoparticles, Composites materials, PKSAnp, Interfacial reaction and DLF-SCM

Novel Multifunctional PKSAnp/A356 alloy composites Synthesis by DLF-SCM

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ABSTRACT

The interfacial reaction of novel multifunctional composite of palm kernel shell ash nanoparticle(PKSAnp)-A356 alloy produced by double layer feeding-stir casting method (DLF-SCM) was studied. The composite was produced using 0 and 4wt%PKSAnp in A356 alloy. X-ray diffractometer(XRD), transmission and scanning electron microscopes were used for the analysis. It was observed that DLF-SCM increased the wettability of the PKSAnp in A356 alloy and decreased the brittle intermetallic phase. There was a uniform distribution of the PKSAnp in A356 alloy. The mismatch at the interface between the PKSAnp and A356 alloy was 4.26%. The Al phase and the PKSAnp are parallel in relationship along the interfaces. Dislocation structure at the interface was visible and coherent interface with regular arrangement of PKSAnp was observed.

Keywords: Nanoparticles, Composites materials, PKSAnp, Interfacial reaction and DLF-SCM

Abstract ID: 665

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Advances in the Synthesis and Characterization of low dimensional, nano and 2D materials

Keywords: Graphene, Mechanical Testing, Large Scale, Thin Films

Fracture Strengths of Centimeter-Scale Monolayer Graphene Films

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Fracture strength measurements of graphene had been reported at microscale.¹ We invented a method to transfer centimeter-scale ultrathin films onto custom-designed substrates for mechanical testing, and were able to use it to obtain Young's modulus and fracture strength of monolayer CVD-grown graphene films.² (This new method allows tensile testing of macroscale (centimeter or larger) graphene single layer (or multilayer) films—essentially anywhere in the world as almost all universities are outfitted with a dynamical mechanical analysis (DMA) testing system similar to the one we used in our tensile loading experiments.) Traditional methods for transferring single layer graphene films involve dissolving or 'peeling' support layers like PMMA; we deposited camphor to generate a micron-thick "supporting molecular film". Large-area ultrathin films could be transferred onto hollow substrates without damage. The camphor is then trivially removed—it simply sublimates away and thus undesirable stresses are avoided on the as-transferred films. Tensile tests were carried out on samples of graphene supported by a ~100 nm thick polycarbonate film; graphene stiffened this sample significantly, thus its intrinsic mechanical response could be extracted. Polycrystalline graphene film had Young's modulus values ranging from 637 GPa to 793 GPa and fracture strengths ranged from 3.17 GPa to 3.53 GPa. 'Highly oriented' (they are essentially single crystal) graphene grown on single crystal Cu(111) foils has long 'folds' present, and this allowed configuring samples with the folds parallel, or alternatively perpendicular, to the tensile loading direction. The modulus values ranged from 683 to 775 GPa for single crystal graphene (folds orthogonal) and between 728 and 908 GPa (folds parallel). The fracture strengths ranged from 3.82 GPa to 5.45 GPa (folds parallel). Thus, macroscale CVD graphene that we have tested to date has strengths smaller than the highest strength carbon fibers made by Toray (about 7 GPa) and our method now provides the appropriate test method for addressing the question: how strong can real graphene be at macroscale?

Key Words: Graphene, Mechanical Testing, Large Scale, Thin Films

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Abstract ID: 666

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Plenary

Topics: Anti-cancer therapy

Keywords: Betaine-HCl; MNPs; Hyperthermia Application; Cytotoxicity; SAR

Highly water-dispersible Betaine-HCl Functionalized Co_{0.5} Zn_{0.5} Fe₂ O₄ magnetic NPs for hyperthermia application

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Co_{0.5}Zn_{0.5}Fe₂O₄ nanoparticles (CZF NPs) functionalized with oleic acid (OA) was synthesized using a chemical Coprecipitation method for the potential application in Magnetic Fluid Hyperthermia (MFH). To render hydrophilicity and to increase the colloidal stability of the NPs, they were further functionalized with betaine-HCl (BTH). The magnetic properties and heating ability of these magnetic NPs (MNPs) are investigated. Heating ability of the CZF NPs and BTH-OA CZF NPs was studied under different applied AC magnetic fields of 167.5-335.2Oe at fixed frequency 265 KHz. To study the effect of coating on the surface of CZF NPs, the NPs are characterized X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy. XRD pattern indicated that the CZF NPs were pure cubic spinel structure. The decoration using BTH-OA did not result in a phase change. Transmission Electron Microscopy (TEM) study, confirms reduction in the agglomeration of particles when the MNPs were capped with OA and then BTH. Zeta potential experimental results proved that BTH-OA coated NPs have excellent stability in aqueous solution. The coated MNPs show increase in specific absorption rate value of 133 W/g at 335.2 Oe, making them more suitable for hyperthermia application. In addition, these functionalized CZF NPs are biocompatible with L929 cell lines and do not have toxic effects for further in vivo use.

Abstract ID: 667

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Photonic and optoelectronic device applications of low dimensional, nano and 2D materials

Keywords: Organic Laser, Laser Display, 3D Printing

Organic Printed Microlaser Arrays

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Exploring a universal technique for the manufacture of reproducible organic material geometries in large quantities, just as photo-lithography is to the traditional silicon-based electronics and photonics, is essential for the upcoming flexible integrated photonics. We developed a solution printing strategy for the function-directed controllable and rapid fabrication of high-quality organic microlaser arrays, which was subsequently applied as the building blocks of the panels of organic laser displays and as the elements of photonic integrated circuits. The printed soft photonic systems show competitive performances with their nowadays silicon-based counterparts; and moreover, they even take advantages of mild processing, flexible doping, active/responsive characteristics, etc.

Abstract ID: 668

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Invited Talk

Topics: Immunomodulatory biomaterials

Keywords: Immune tolerance, nanoparticles, immunosuppression, immunotherapy

Use of Polymeric Nanoparticle Platform to induce Treg-mediated Antigen-Specific Immune Tolerance

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Nanoparticles can be used to accomplish antigen-specific immune tolerance in allergic and autoimmune disease. The available options for custom-designing tolerogenic nanoparticles (NPs) include the use of nanocarriers to promote tolerance to self or foreign antigens. Here, we demonstrate the engineering of a biodegradable polymeric poly(lactic-co-glycolic acid) (PLGA) nanocarrier for the selective delivery of the murine allergen, ovalbumin (OVA) to the immune system. This was accomplished by developing a series of NP in the 200-300 nm size range as well as decorating particle surfaces with ligands on professional tolerogenic endothelial cells (ECs). ECs represent a major antigen presenting cell type that is capable of generating regulatory T-cells (Tregs). Ex vivo EC exposure to NPOVA resulted in abundant TGF- β , IL-4 and IL-10 production, which was further increased by surface ligands. Additional animal experiments showed that for the chosen NP size range, OVA was almost exclusively delivered ECs by surface ligands. Moreover, prophylactic treatment with NPOVA in OVA-sensitized and inhalation challenged animals could be seen to significantly suppress or eliminate anti-OVA IgE responses, airway eosinophilia and TH2 cytokine production in the bronchoalveolar lavage fluid. The suppression of allergic airway inflammation was further enhanced by surface ligation, which induced high levels of TGF- β production in the lung along with the appearance of FOXP3⁺ Tregs. The NPs could also interfere in allergic airway inflammation when delivered post-sensitization. These data indicate that the engineered uptake of PLGA NP can be used for tolerogenic immunotherapy in allergic airway disease, with the promise of treating additional allergic or autoimmune disorders.

Abstract ID: 669 / Poster: 26

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Biosensors for Imaging

Keywords: Fluorescent Probe, Biosensing, Bioimaging, Aggregation Induced Emission

Specific Detection and Visualization of Cyclooxygenase-2 by a Targeted Fluorescent Probe with Conformation-Induced Light Up Activity

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The precision medicine initiative aims to use advances in basic and clinical research to develop therapeutics that selectively target and kill cancer cells. Under the same doctrine of precision medicine, there is an equally important need to visualize these diseased cells to enable diagnosis, facilitate surgical resection, and monitor therapeutic response. Molecular fluorescence imaging has become a powerful tool in cancer diagnosis and clinical surgery, because it emerges as a promising noninvasive, real-time, high-sensitivity and low-cost imaging technique.¹ One such breakthrough that is likely to have a broad impact on imaging techniques is the development of targeted fluorescent probes that enable imaging cancer cell with high selectivity and sensitivity.²⁻³ Here we present a successful example of a fluorescent light up probe for specific biomarker sensing and imaging. Cyclooxygenase-2 (COX-2) was chosen as a specific analyte, because it is an attractive target for molecular imaging because it is normally absent from cells and is greatly upregulated in many premalignant and malignant tumors and inflammatory lesions. Indomethacin (IMC), a selective inhibitor, serving as the recognizing moiety of fluorescent probe to target COX-2 was reported by Marnett et al and Peng et al previously. Considering the high affinity and specificity of IMC to COX-2, we integrated IMC moiety with one 9,10-diatrylanthracene (DSA) derivate unit, a typical AIE fluorogen,⁴ and achieved a high brightness, high selectivity of fluorescent light up probe (NDSA). The NDSA showed very weak emission in the buffer solution, while boosted strong fluorescence when it bound to COX-2 due to the restriction of intramolecular motion (conformation change) mechanism. The unique responding mode of NDSA allows the highly selective detection and visualization of COX-2 and enables the discrimination of cancer cell or tumor, suggesting a potential candidate for early diagnoses of disease.

Abstract ID: 670

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Carbon Nanomaterials

Keywords: Quantum Chaos, RMT, the K@C20@C80 nano-onion billiard

Quantum Chaos in the K@C20@C80 nano-onion billiard

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The exact calculations of the K@C20@C80 nano-onion billiard random matrix theory are provided here which should lead to a better interpretation of quantum chaos. We show that band electrons in the K@C20@C80 nano-onion billiard are in highly chaotic quantum state. The random matrices Gaussian orthogonal and Gaussian unitary ensembles are discussed for the K@C20@C80 nano-onion. Our results are different for both cases. The distribution of the smallest singular value for the GOE and GUE distribution of the K@C20@C80 nano-onion billiard illustrated so that the band chaos is quantum origin. Each approach indicated its own definition of the spectral curve, a geometric object encoding all the properties of a model. This paper shows how important the role of energy levels is with regard to the structure of the model. The results are shown that there are chaotic behaviors for a total energy, demonstrating chaotic appearance according to K@C20@C80 nano-onion oscillators in mechanical systems of nanoscaled.

Abstract ID: 671

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Computational studies of Biomaterials

Keywords: DFT, Antidiabetic Drugs, Conformational Search, Dipole Moment, Homo-Lumo

Determination of electronics and molecular structure of Nateglinine antidiabetic drugs using DFT

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Diabetes mellitus is a metabolic disease which is characterized by high blood glucose level and result from defects in insulin secretion, insulin action or both. Gaussian09 software package which uses Density functional theory was used to search for conformers, optimize the structure, and calculate the electronic properties of the Nateglinide anti-diabetic drugs. It was found that, C20-C18-C16-H45 isomer has the lowest energy of -2762.448518 eV and transition energy of 400.8615826 eV. Also it was found that dipole moment increases as the basis set increases while the total energy decreases. Information on bond length, bond angle and dihedral angle of the optimize structure was reported. Finally the Homo-Lumo formations reveals that there are more free non bond electron in the homo site due to higher ionization potential.

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Thursday, 22/Aug/2019 11:00am - 11:12am

Abstract ID: 672 / FTF: 1

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin Films in Biological and environmental Applications

Keywords: Layered double hydroxide, Nanoclay, Thin Film

Tailoring the properties of polyamide thin film membrane with layered double hydroxide nanoclay for enhancement in water separation

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This current paper presented a new candidate and potentially to improve the current membrane materials in water filtration process. With that, the primary materials used in this research study is layered double hydroxides (LDH) nanoclay which can be obtained from earth minerals and self-synthesized from inorganic salts that were thoroughly discussed to help a better understanding of these materials. The current technologies of water separation was still lagging behind and ineffective especially in removal of divalent metal ions and multivalent salts. Infeasibility of reverse osmosis membrane made it not a viable option for divalent salts filtration. With that, nanofiltration (NF) membrane offered as an alternative to substitute available method. In this study, thin film nanocomposite (TFN) membranes was fabricated by incorporating layered double hydroxides (LDH) nanoclay. The LDH nanoclay with different loading ratio of 0, 0.05, 0.1, 0.15 and 0.2 were impregnated into polyamide layer on top of polysulfone substrates. The fabricated TFN were characterized in terms of physicochemical properties (SEM and FTIR) and membrane hydrophilicity (contact angle). After the addition of LDH, the morphological structures of TFN membranes were changed and the surface hydrophilicity was enhanced significantly. FESEM images displayed a typical ridge and valley morphology with nodule-like structures. As the LDH loading was increased, the contact angle decreased from 50.56° to 29.76° showing the surface hydrophilicity of membrane is improved. The separation performance of membrane was evaluated in terms of salt rejection ability (Na₂SO₄) by cross flow filtration system. The best performance NF membrane was (TFN 0.05) with high water flux and MgCl₂ rejection with values of 27.18 L/m².h and 95.98% respectively. This study has experimentally validated the potential of LDH materials in membrane process for improvement in water separation process.

Abstract ID: 673

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Bio-inspired design of composites

Keywords: Honeycomb, Biomimetic Design, Composites, Sandwich Structures

Honeycomb structures: how accurate does Nature, and indeed engineering, have to be?

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In 1859, Charles Darwin considered the hive-bee honeycomb as being ‘an absolutely perfect structure, economising labour and wax’. Beyond the hive-bee, the hexagonal honeycomb system is ubiquitous in nature, and has been adopted within engineering to resist out-of-plane compressive and shear loads. The in-plane properties of honeycombs are far less stable in compression and shear than their out-of-plane properties, as there is less material to resist load in a single direction. A primary benefit in using honeycomb structures is that they have desirable specific stiffness and strength properties. They are for this reason, used in lightweight mechanical materials technologies and been very successful in several industrial sectors. Nevertheless, not all versions of natural honeycomb structures in Nature are perfectly organised. Very often, there are variations in size, shape and layup. Sometimes, the hexagonal system becomes a combination of hexagonal, trigonal and pentagonal primitives. Sometimes, they lose the distinctness of their edges and become somewhat more circular. This paper concerns the in-plane properties of honeycombs. Using finite element analysis methods, coupled to 3D printing and mechanical testing, we map the variations in properties of honeycomb structures as a function of induced defects.

Abstract ID: 674

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Anti-cancer therapy

Keywords: Liposomes; Wheat germ agglutinin; Cisplatin; MiaPaca-2 cells

Cisplatin loaded lectinized liposomes system for nuclear targeting

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The aim of this study was to design an engineered/lectinized drug delivery system for the nuclear targeting of anticancer drug (cisplatin). Liposomal formulation was developed by the thin film hydration method and modified with Wheat germ agglutinin (WGA) lectin. The cisplatin loaded plain(NCL)and WGA modified(WCL) liposomal formulation were optimized by design of Experiment (DoE) and characterized for chemical structure, particle size(PS), polydispersity index, Zeta Potential, drug entrapment efficiency, and WGA lectin coupling efficiency. Surface morphology of optimized formulation was studied by using Transmission Electron Microscopy, Atomic Force Microscopy, and Confocal Laser Scanning Microscopy. The PS of the prepared formulation was found to be 154 ± 6.45 nm and 183.5 ± 0.024 nm, with the negative value of zeta potential respectively for formulation NCL and WCL while EE % was $83.5 \pm 2.1\%$ and $79.2 \pm 3.1\%$. In addition In Vitro drug release profile of developed formulations reveals a typical biphasic pattern with a burst release of drug at initial stage followed by sustained release of the drug. The Ex- vivo study of liposome formulations was performed on human MiaPaca-2 pancreatic cancer cell line & confirms the nuclear targeting of WCL formulation. The data clearly suggested that the release of drug from optimized liposome was sustained with less cytosolic distribution, and appeared to reach the nucleus selectively of MiaPaca-2 cancer cells within 3 hours.

Thursday, 22/Aug/2019 11:36am - 11:48am

Abstract ID: 675 / FCM-3: 4

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Biocomposites

Keywords: Bioactive, Nano, Resin Infiltration

Innovative bioactive resin infiltrant

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Innovative bioactive resin infiltrant

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Integrating nano hydroxyl apatite particles in resin infiltrant is a promising route for treatment of dental caries. This study is aimed to assess the effect of nanohydroxy apatite incorporation into the resin infiltrant on its properties. Materials and methods: The total sample size in the three groups was 30 specimens (ICON, ICON + 5% NHA, ICON + 10% NHA). The specimens were randomly allocated in three test groups. Water sorption and solubility were measured as defined by ISO 4049 specification. The color stability specimens were evaluated with spectrophotometer to record the CIE L*a*b* parameters of the specimens. Color change was calculated to determine the extent of color stability between the tested groups. Results: There was a statistically significant difference between the groups regarding to the water sorption, solubility and the color stability. Conclusion: This study offers a promising route to greatly enhance resin infiltration treatment regarding its durability and color stability

Key Words: Bioactive, Nano, Resin Infiltration

Abstract ID: 676

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin Films in Photovoltaic Cells and Energy

Keywords: ZnTe thin films, Vacuum Coating, Energy band gap, Resistivity, XPS study

Pronounced impact of Te-enrichment on physical properties of ZnTe thin films for solar cell applications

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Closed space sublimation (CSS) technique was used to deposit thin films of zinc telluride (ZnTe) on glass substrate. Tellurium (Te) was deposited on to the as-deposited thin films of ZnTe with subsequent annealing using CSS as a next step. X-ray diffraction (XRD) results showed before and after enrichment the preferred orientation is [111] having cubic phases. The crystallite size was found to be increased in Te enriched ZnTe samples. The scanning electron microscope (SEM) was used to analyze surface morphology. For Te-enriched samples the average grain size is greater than as compare to as-deposited ZnTe thin films. In order to confirm the compositions of Te and Zn in ZnTe films energy dispersive X-rays (EDX) was used. The Te-enriched samples have less optical transmission in UV-VIS-NIR range as compare to the as-deposited ZnTe thin films. A very small change in optical band gap energy was observed in Te-enriched ZnTe thin film samples. Four point probe technique was used to study electrical properties of as-deposited and Te-enriched ZnTe thin films. These results show that the as-deposited samples has resistivity of 106 Ω -cm while for Te-enriched samples resistivity decreases to 104 ohm-cm. XPS study has been carried out for chemical states and bonding which confirmed the excess Te contents in ZnTe thn films. These shows that Te-enriched samples are suitable for back contact of II-VI solar cells.

Abstract ID: 677

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Solar Cells

Keywords: Perovskite, Lead free, Copper oxide

Device Modeling for High Efficiency Lead Free Perovskite Solar Cell with Cu₂O as Hole Transport Material

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In recent years, organic-inorganic metal halide perovskites have attracted significant attention as absorber materials for solar cells, owing to their excellent optoelectronic properties, low cost of fabrication and high photovoltaic performance [1]. In most of the conventional perovskite ($E_g \sim 1.6$ eV) solar cells, $APbX_3$ ($A = CH_3NH_3^+$, $HC(NH_2)_2^+$, Cs^+ , Rb^+ ; $X = I^-$, Br^- , Cl^-) is used as the active layer for absorption of incoming sunlight [2, 3]. However, the well-known toxicity of lead (Pb) poses serious concerns regarding the possible health and ecological hazards [1]. Hence, in order to avoid toxicity, $CH_3NH_3SnI_3$ is being used here as the absorber material having a direct bandgap of 1.30 eV. In this work, Cu_2O is employed as the hole transport material (HTM) and PCBM as the electron transport material (ETM). The proposed perovskite solar cell device is explored using inverted planar (p-i-n) type structure which is more desirable due to its less current hysteresis, low temperature and simple fabrication process [4]. In this device simulation, $Cu_2O/CH_3NH_3SnI_3$ and $CH_3NH_3SnI_3/PCBM$ interface defect layer (IDL) are also incorporated in order to take into account the effect of interface recombination on the final device performance. In both bulk and interface materials, defect type of neutral charge is considered to be Gaussian with the capture cross-section for both electrons and holes of $2 \times 10^{-14} \text{cm}^2$. Moreover, the reference for defect energy level (E_t) is considered to be above E_i , the energy level with respect to reference as 0.6eV with characteristic energy at 0.1eV and the total density of defects (N_t) in the perovskite materials and interface materials are taken as $2.5 \times 10^{13} \text{cm}^{-3}$ and $1 \times 10^{18} \text{cm}^{-3}$ respectively. The numerical simulation of the designed solar cell is done using three basic equations i.e. Poisson's equation, carrier continuity equation and drift-diffusion equation. The parameters which affect the overall performance are investigated and found that absorber thickness, doping concentration of both HTM and ETM and thickness of Cu_2O influence the solar cell performance. The optimized performance of the perovskite solar cell with efficiency of more than 30%, V_{oc} of 0.99V, J_{sc} of 35.12mA/cm² and FF of 87.12% are obtained when the thicknesses of perovskite and Cu_2O were 300nm and 10nm respectively and the doping of Cu_2O and PCBM were $9 \times 10^{21} \text{cm}^{-3}$ and $1 \times 10^{21} \text{cm}^{-3}$ respectively. These results indicate that $CH_3NH_3SnI_3$ based solar cell can be a potential choice for future non-toxic and high performance single junction and all-perovskite multijunction photovoltaic applications.

Abstract ID: 678

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin Films in Photovoltaic Cells and Energy

Keywords: GLAD, Nanoparticles, Nanowires, Plasmon, TiO₂

Investigation of Au Nanoparticle assisted TiO₂ Nanowires for Solar Cell Applications

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Titanium Dioxide (TiO₂) NWs have been explored in many optoelectronic device applications [1-2], due to their favorable properties like photocatalytic, large surface area, decoupling of light absorption and direct electron conduction pathway to conductive substrate [3-4]. However, only ~5% of energy can be absorbed from the solar spectrum due to large band gap of TiO₂ [5]. Because of this reason many researchers are trying to enhance the photocatalytic properties of TiO₂ in visible region by metal and non-metal doping and chemical modifications. Recently, plasmon sensitized photo activities of TiO₂ have become more attractive due to their size dependent photon energy absorption in solar spectrum [6]. The metal nanoparticles are considered to have better photostability as compared to semiconductor quantum dots which usually experience anodic photo corrosion. Therefore, this research work is an attempt to synthesize gold (Au) nanoparticles (NP) assisted vertically oriented TiO₂ nanowires (NWs) photoanode using Glancing Angle Deposition (GLAD) technique on Si substrate [1]. The FE-SEM analysis manifests the successful growth of Au-NP-TiO₂-NW on the substrate. And, the TEM image of a typical NW confirms the presence of Au NP at the mid of the TiO₂ NWs. The optical absorption spectrum of annealed Au-NP-TiO₂-NW sample manifests that the absorption of photons is extended toward the visible region due to multiple scattering of light inside the vertical NWs which in turn enhance the Surface Plasmon Resonance (SRP) effect of Au NPs. The photoluminescence (PL) analysis of Au-NP-TiO₂-NWs sample shows a broad peak with an emission peak at ~389 nm (3.19 eV) which is from the main band transition and the origin of blue light emission at ~453 nm (2.73 eV) may be due to sub-band gap transition originated from the oxygen vacancies. This simple and cost effective controllable metal NP assisted NWs growth technique without using any template may be applicable for fabrication of photoanode to enhance the solar cell efficiency.

Abstract ID: 679

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Anodes and cathodes Materials

Keywords: NiO nanoparticles, Calcination, Cyclic voltammetry, Galvanostatic charge/discharge, Electrochemical

Supercapacitor studies on nickel oxide nanoparticles prepared by facile route calcination

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Nickel oxide with high theoretical capacity of about 718 mAh/g, high chemical and thermal stability, low cost, and environmental benignity has attracted enormous attention as anode materials for lithium ion batteries [1-3]. NiO with various structures such as nanopowders, microsphere, nanosheets, nanoflakes, microtubes and etc have been developed to achieve high reversible capacity, enhanced cycling performance and good rate capability [4,5]. NiO can be prepared by various techniques such as microwave route, spray pyrolysis, sol-gel, heat treatment, calcination and hydrothermal [6,7]. There are several reports on the pseudocapacitive performance of different NiO based nanostructures, with a specific capacitance from 250 to 950 mAh/g [1]. For example, Vijayakumar et al., reported maximum specific capacitance of 401 mAh/g at a current density of 0.5 mAcm⁻¹ for NiO nanoflakes prepared using microwave route [7]. NiO microtubes obtained by calcination of Ni(DMG)₂ exhibit maximum specific capacitance of About 640 mAh/g after 200 cycles at 1 A/g [5].

In this study, we report synthesis of NiO nanoparticles using the facile route of calcination and characterized by FT-IR, XRD and TEM. Also, the electrochemical performance of NiO nanoparticles has been reported and discussed.

Abstract ID: 680

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Lithium Ion Batteries

Keywords: Solid state Li -ion batteries, Active materials, Prototype cells

Solid State Li-ion Battery Research: C-MET Initiative and Future Plans

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Lithium batteries are characterized by high specific energy, high efficiency and long life. These unique properties have made lithium batteries the power sources of choice for the consumer electronics market with a production of the order of billions of units per year. These batteries are also expected to find a prominent role as ideal electrochemical storage systems in renewable energy plants, as well as power systems for sustainable vehicles, such as hybrid and electric vehicles.

In order to develop the Li-ion battery technology indigenously, C-MET has initiated and actively working for the development of Active materials (cathode and anode) and has been developed an entire battery fabrication and testing facility for the button/coin type and pouch / rectangular cells under one roof. The development of materials for high energy batteries is a continuous process and C-MET is working for the development of novel materials for the high charge capacity and energy density. The facility has already been created for the large scale synthesis of active materials (500 gm batch level) using spary dryer (Fig. 1 a). Lithium titanium oxide (LTO) as an anode material has been synthesized via solid-solid combustion process. The nanostructured spherical hard carbon (anode material) has been synthesized using novel natural sources (potato, banana and sweet potatoes) and one Indian patent have been filed based on this invention.

These developed cathode and anode materials were compared with the commercially available active materials (Aldrich and MTI, Corporation USA make) and fabricated a prototype button/coin (2032 type) cells. Fig.1 b shows the prototype of coin cells fabricated using the active materials developed by C-MET. The electrochemical performances of these cells are found to be similar to that of the commercially available active materials.

We have successfully developed thin, flexible & light weight batteries and also working for the development of polymer based electrolyte for Li-Polymer batteries. We have also initiated the activities for the development of Li-Air and Na -ion batteries for the hybrid/electric vehicles for smart, green & clean transportation.

Abstract ID: 681

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Nanomedicine, Nanobiotechnology, Environment and Nanotoxicology

Keywords: Calcium hydroxide; Genomic instability; Mitochondrial DNA damage and mice; Nanoparticles

Genomic instability 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 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 and MDA levels and decreased SOD and Gpx activities reversely proportional to Ca(OH)₂ particles size in the liver, brain and bone marrow tissues. 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: Ca(OH)₂ induced genomic instability is based on tissue type and particle size and mediated through the impairment of mitochondrial DNA and increases the ROS generation that exhausted the antioxidant defense in the brain and bone marrow tissues.

Abstract ID: 682

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Fuel Cells

Keywords: Fuel cell, Nanomaterial, Polymer electrolyte membrane

Improving properties of Polymer electrolyte membranes for fuel cell applications - Role of nanostructured materials

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Polymer electrolyte membrane fuel cell has been considered as an alternative type of fuel cell compared to its liquid electrolyte counterpart. This is due to the membrane multifunctional ability of the membrane electrolyte. The triple role of the membrane include (i) charge carrier for ions, (ii) avoid fuel crossover/permeability, and (iii) electronic insulator to prevent parasitic losses due to passage of electrons through the membrane. Unfortunately the Polymer electrolyte membranes still suffers from fuel crossover/permeability, low ion conductivity and dehydration during operation. To address these challenges, nanostructured materials such as, carbon nanotubes, TiO₂, ZnO, nanofibers, graphene oxide have been integrated in the polymer matrix to form a nano-enabled composite membranes. The membranes fabricated in this study were found to have improved basic properties for fuel cell application; methanol crossover reduced, ion conductivity increased and water hydration improved, which lead to an enhanced peak power density. This study offers a promising route to greatly enhance the polymer electrolyte membrane properties and provides insights on the influence of nanostructured materials on the electrolyte membrane for fuel cell application.

Abstract ID: 683

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Applications of Composites

Keywords: Metal-organic Framework, Carbon, Battery

Transition Metal Sulfides Based on Graphene for Electrochemical Energy Storage

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Transition metal sulfides, as an important class of inorganics, can be used as excellent electrode materials for various electrochemical energy storages, such as lithium-ion batteries, sodium-ion batteries, supercapacitors and others. Recent works have identified that mixing graphene or graphene-derivatives with transition metal sulfides can get novel composites with better electrochemical performance. This review summarizes the latest advances on transition metal sulfide composites with graphene or graphene-derivatives. The synthetic strategies and morphologies of these composites are introduced. We then discuss their applications in lithium-ion batteries, sodium-ion batteries and supercapacitors. Finally, we give our personal viewpoints about the challenges and opportunities for the future development about this direction.

Abstract ID: 684

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Electrocatalysis

Keywords: Ultrathin nanosheet, Metal-organic framework, Assemblies, Ascorbic acid, Electrocatalysis

Ultrathin Nanosheet Ni-MOF Assemblies for High-Efficiency Ascorbic Acid Electrocatalysis

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Owing to unique porous structure, metal–organic framework (MOF) nanosheets are considered one of the best active materials for high-performance electrocatalysts. Ultrathin nanosheet Ni-MOF assemblies, $[\text{Ni}_3(\text{OH})_2(\text{C}_8\text{H}_4\text{O}_4)_2(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$ were synthesized by a simple solvothermal method and used to efficiently catalyze ascorbic acid (AA) in a common phosphate buffer solution (PBS, pH=7.2). Electrochemical data analysis revealed good catalytic activity performance and outstanding stability for the ascorbic acid oxidation reaction. The reason for analyzing its intrinsic may depend on the structure of the ultrathin nanosheet. This structure not only provides a pathway for improving electrocatalytic performance, but its special aggregation state also makes it more stable in electrocatalytic AA.

Abstract ID: 685

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Piezotronics for smart systems

Keywords: piezoelectric ultrasonic motor, second-order bending mode, FEA, low driving voltage

Design and experiments of an eight-zonal piezoelectric tube-type threaded ultrasonic motor

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In order to reduce the driving voltage and gain better output characteristics of the piezoelectric actuators, an eight-zonal piezoelectric tube-type threaded ultrasonic motor based on two second-order bending modes was analyzed using the method of finite element analysis (FEA), and a prototype was fabricated and experimentally studied in this research. This piezoelectric motor is designed to be excited by four electrical sources applied to four groups of electrodes on the customized lead zirconate titanate (PZT) tubular stator (inside diameter 5.35 mm, outside diameter 6.35 mm, length 30 mm) simultaneously, with $\pm 90^\circ$ phase shifts between adjacent electrodes. Experimental results show that the threaded motor can output a stall pulling force of about 5.0 N and a linear velocity of 4.9 mm/s with no load at the driving voltage of 40 Vpp. The prototype consists of just a PZT tubular stator, two nuts attached to the stator and a threaded rotor. This piezoelectric motor with compact structure and screw drive mechanism shows a relatively fine velocity controllability, and have huge superiority in micro-positioning systems.

Thursday, 22/Aug/2019 8:24am - 8:36am

Abstract ID: 686 / FESC: 3

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: Flexible supercapacitor, Machine-washable, Composite, Energy Storage

Machine-washable flexible supercapacitors based on laminate composites

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Flexible and wearable supercapacitors have been intensively studied recently because of their potential as safe and durable rechargeable energy sources for future wearable electronics. However, flexible supercapacitor prototypes reported so far have not shown sufficient mechanical properties that could withstand critical situations which are common for daily attires, such as folding, twisting, and machine washing.

Here we demonstrate flexible supercapacitors that are foldable, twistable, and machine-washable due to exceptional mechanical properties of the materials. The devices are constructed using thin laminate composites of activated carbon fiber, glass fiber, and bio-safe polymer electrolyte. The prototypes show adjustable areal capacitances of over 50 mF/cm², and almost unchanged performance after being folded, twisted, and washed together with regular garments in a washing machine for a full washing cycle. The excellent electrochemical performance, flexibility and mechanical durability make the flexible supercapacitors promising to be integrated with daily garments to power various wearable electronics.

Abstract ID: 687

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Catalyst Modelling and Simulation

Keywords: Density functional theory, titanium dioxide, anatase, brookite, polaron

Density functional theory study on polaron formation of Anatase and Brookite TiO₂ using hybrid functional and DFT+U methods

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Anatase and brookite are robust materials with enhanced photocatalytic properties. In this study, we present electron and hole polaron geometries and their energetics using density functional theory (DFT) with hybrid functional and the Hubbard on-site potential methods for anatase and brookite. Hybrid functionals predicted there is no localized electron and hole polaron formation in anatase. On the contrary, brookite formed both electron and hole polarons. Brookite electron polaronic solution has localized and delocalized states coexist. Hole polarons are dispersed mainly on two coordinated oxygen ions. Hubbard on-site potential is tested for a wide range from 4.1 eV to 10 eV and found brookite polarons are formed at $U = 6$ eV and anatase polarons formed at $U = 8$ eV. Brookite electron polaron always localized on a single titanium ion under Hubbard model, whereas hole polaron is dispersed on four oxygen atoms as in the case of hybrid DFT studies. Anatase electron polarons dispersed at lower on-site potential but more localized with higher potential. From both the methods, it is predicted brookite has a higher driving force to produce polarons than that of anatase.

Acknowledgements

This study was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT and Future Planning (No. NRF-2017R1E1A1A01074266). This research was supported by the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT & Future Planning (No. NRF-2015M1A2A2057129 and NRF-2016M1A2A2937151).

Abstract ID: 688

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Invited Talk

Topics: Antimicrobials

Keywords: Silver Nano particle, PVP, Antimicrobial, Electrical Properties, Optical Properties

Nano-biomaterials in Antimicrobial Therapy

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Silver nanoparticles (AgNps) have attracted much interest in biomedical engineering, since they have excellent antimicrobial properties. Silver nano polymer composites have applications in biochemical sensors, antimicrobial activity and drug delivery system. Silver nanoparticles are more effective than ionic homologues (Ag⁺) for their antimicrobial activity.

Polymer matrices have been frequently used as particle stabilizers in chemical synthesis of metal colloids since these prevent agglomeration of the particles. Novel hybrid material thin films based on various polymeric systems with embedded silver nanoparticles were synthesized using various methods. Among them, polyvinylpyrrolidone (PVP) attracts considerable attention because of its excellent chemical and physical properties making it a good polymeric material as a coating or as an additive to different materials. Further, PVP has received special attention because of its high chemical stability, no toxicity and excellent solubility in many polar solvents.

The Electrical, optical and plasmonic response of Ag Nps onto thin layers of polymer composites show encapsulation of nanoparticles.

The method of preparation of the nano silver PVP composite is very important in the sense of antimicrobial and biocompatibility properties of the thin film. The preparation of PVP/P4VP blends by evaporation of silver in vacuum of the order of 10⁻⁶Torr is a significant method.

Here, the antibacterial activity of AgNps/polymer composites against various common bacteria is discussed. The antibacterial activity of the synthesized hybrid materials were tested against various bacteria, commonly found in hospital environment. Silver nano structures have especially been of interest because of contrast agents for biomedical image. Shunts used for hydrocephalous silicon elastomeric grafted with hydro gel, Poly vinyl pyrrolidone (PVP) soaked in various antibiotics proved to be active for longer time.

Abstract ID: 689

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

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

Keywords: low-dimensional, negative capacitance effect, short-channel effect, subthreshold swing

Negative Capacitance Field-Effect Transistors with Subthreshold Swing below the Physics Limit

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Boltzmann distribution of electrons induced fundamental barrier prevents subthreshold swing (SS) from less than 60 mV/dec at room temperature, leading to high energy consumption of MOSFETs. Herein, we demonstrate that an aggressive introduction of negative capacitance (NC) effect of ferroelectrics can decisively break the fundamental limit governed by the “Boltzmann tyranny”. Thus the operation voltage of the whole integrated circuits maintain a high level. Lowering the SS of the transistors is an efficient approach for low-power circuits, especially for short-channel electronics. Herein, by introducing a ferroelectric P(VDF-TrFE) in the gate dielectric layer stacks, the SS values of the transistors are below 60 mV/dec at room temperature, which is benefit from the negative capacitance effect of the ferroelectric layer. We have demonstrated SS value of 42.5 mV/dec in MoS₂ NC-FETs, and simultaneously achieve superior performance of a transconductance of 45.5 $\mu\text{S}/\mu\text{m}$ and an on/off ratio of 4×10^6 with channel length less than 100 nm. Moreover, to fully take the advantages of the efficient geometry of nanowire (NW) and the high mobility, side-gated In₂O₃ NW NC-FETs are assembled, which exhibits high saturation current density of 550 $\mu\text{A} \cdot \mu\text{m}^{-1}$ and SS ≤ 60 mV/dec for over 4 decades of channel current. The assembled inverter circuit can demonstrate the impressive voltage gain of 25 and cut-off frequency of over 10 MHz. By utilizing the self-aligned fabrication scheme, the device can be ultimately scaled down to below 100 nm channel length. The devices with 200 nm channel length exhibits the best performances, in which a high on/off current ratio of $>10^7$, a large output current density of 960 $\mu\text{A} \cdot \mu\text{m}^{-1}$ and a small SS value of 42 mV dec⁻¹ are obtained at the same time. Therefore, the NC-FETs enable fundamental applications through overcoming the Boltzmann limit in nanoelectronics and open up an avenue to low-power transistors needed for many exciting long-endurance portable consumer products.

Thursday, 22/Aug/2019 2:00pm - 2:15pm

Abstract ID: 690 / FLNM-3: 1

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: 2D Topological Materials

Keywords: 2D Topological materials, Monolayer antimonene, 2D superconductor-topological insulator

Epitaxial Growth and Properties of 2D Topological Antimonene and Heterostructures

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The novel properties of graphene honeycomb structure have spurred tremendous interest in investigating other two-dimensional (2D) layered structures beyond graphene for nanodevices. In this talk, I will mention the fabrication and properties of several 2D materials such as graphene, such as, silicene[1], germanene[2], hafnene[3] and topological antimonene with flat or undulated configuration [4], wherein silicon (germanium, hafnium or antimony) atoms are substituted for carbon atoms in graphene. Besides mono-elemental 2D atomic crystals, bi-elemental 2D materials, such as magnetic VSe₂ monolayer[5], semiconducting PtSe₂ monolayer and its intrinsically patterns [6,9], and superconductor transition-metal-trichalcogenide (HfTe₃)[7], grown by direct selenization/tellurization of the Pt/Hf substrate, as well as their application exploring in nanoelectronics and valleytronics will also be introduced. In addition, the stacking heterolayers based on several these kinds of 2D materials, for instance, a superconductor-topological insulator layered heterostructure (with a HfTe₃/HfTe₅ layered configuration) for Majorana bound states will be also presented [8]. The precise structural configurations at atomic-resolution of these materials will also be introduced, based on the measurements by several advanced techniques like LEED, STM/STS and STEM.

Abstract ID: 691

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Optical, electrical and magnetic properties of thin films

Keywords: SHI, ZnO, ALD, RTFM, AFM, XRD, UV-Vis., PL, FTIR, RBS

Influence of 120 MeV Ti⁹⁺ ion beam induced modification on structural, optical, and surface morphological properties of nanocrystalline ZnO thin films grown by Atomic Layer Deposition

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Swift heavy ion (SHI) beam induced modifications in properties in oxide materials leads to have curiosity for evaluating the defects and damage in their physical and chemical properties. Our study systematically introduced the defects in ALD grown ZnO thin films by swift heavy 120 MeV Ti⁹⁺ ion beam irradiation with the range of fluence 5E11 to 1E13 ions/cm² and investigated their structural, magnetic, optical and topographical properties. Room-temperature ferromagnetism was carried out in controlled manner to analyze the variation of significant magnetization with increasing the ion fluence. The results from Atomic force microscope analysis showed the change in grain size and RMS roughness of the virgin and irradiated thin films. Further, the complete statistical description of surface roughness was analyzed by power spectral density (PSD). Ordered arrangement of reflection plane and effect of swift heavy ion irradiation on crystalline structure of thin films were investigated by X-ray diffraction technique (XRD). Moreover, the structural parameters such as stress and strain of virgin and irradiated ZnO thin films were determined using XRD results. The variation in induced stress can be due to the strong density of dislocations defects. An enhancement of the optical properties i.e. absorbance, transmittance and optical band gap of virgin and Ti ion irradiated samples were also observed. Photoluminescence (PL) spectroscopy was employed to investigate PL emission characteristics of the ZnO thin films, as well as the changes induced in intensity of PL emission bands by irradiation of high energy ions. Rutherford backscattering spectrometry (RBS) was carried out to determine the composition and thickness of virgin and irradiated ZnO thin films. ZnO thin films were characterized by Fourier-transform infrared spectroscopy (FTIR) to investigate the vibrational properties of the samples.

Abstract ID: 692

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Keynote

Topics: Piezotronics for smart systems

Keywords: Piezoelectrics, flexible, carbon nanofibers, chitosan, barium titanate.

Flexible chitosan-based BaTiO₃ piezoelectric composites

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In recent decades, there has been increasing interest in the development of the so called build block technologies (transducers, actuators and sensors) to enable to implement the "Internet of Everything". In this context, the motivation of this work was the preparation of a bionanocomposite for biocompatible piezoelectric sensors for biomedical applications. Chitosan, which is a polysaccharide with the ability to form films, was used as matrix and particles of lead-free barium titanate, a ferroelectric and piezoelectric material at room temperature, were used as fillers.

The BaTiO₃ particles were synthesized by hydrothermal method during 24 h at 200 °C. The structural characterization by X-ray diffraction (XRD) and Raman spectroscopy allowed us to verify that the particles synthesized at 200 °C showed a well-defined tetragonal crystallographic structure after 24 hours of synthesis. The particles showed uniformed cubic morphology and average size of about 306 nm. The films were obtained by the solvent evaporation method, after dispersing the particles in different proportions, in the chitosan solution. Structural properties (XRD and Raman), morphological (SEM); physical-chemical (mechanical, degree of humidity, solubility in water and contact angle; and dielectric behavior of the films were characterized. The addition of particles improved the mechanical properties of the chitosan films, making them more resistant, elastic and ductile. These films were more resistant to water than pure chitosan films, revealing the interaction between the particles and the chitosan matrix. In relation to the electric behavior of the films, the increase of particles improves the permittivity of the samples five times in relation to the biopolymer material.

The bionanocomposites developed based on chitosan and barium titanate are promising to be used in biomedical devices since they have high mechanical resistance, elasticity, and ductility, as well as have higher resistance to conditions with high degree of humidity. In addition, they are biocompatible and biodegradable, being an excellent alternative to synthetic polymers.

Thursday, 22/Aug/2019 8:00am - 8:15am

Abstract ID: 693 / FCM-2: 1

Symposium 2: Functional Composite Materials (FCM)

Keynote

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

Keywords: Flexible, multifunctional, magnetic hyperthermia, biomaterial

Cytocompatible chitosan-based bionanocomposites with antioxidant, electrically-conductive and superparamagnetic properties

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Multifunctional materials based on the interaction of biological, electronic, and magnetic systems are on the basis of promising emerging technologies. Several biomedical applications such as magnetic resonance imaging, drug and gene delivery, magnetic hyperthermia, and tissue engineering are examples of applications that require the use of biocompatible and tailor-made materials developed under green methodologies.

Here, it is described the development of flexible and multifunctional chitosan-based bionanocomposites with a mixed reduced graphene oxide-iron oxide (rGO-Fe₃-xO₄) filler in different percentages. The filler is prepared by one-pot synthesis, ensuring good dispersibility of the Fe₃-xO₄ nanoparticles with the rGO and, consequently, within the chitosan matrix during solvent casting. The resulting bionanocomposites provide tunable electrical conductivity and superparamagnetic response at room temperature, and antioxidant activity that can be 9 times higher in films with 50% of filler than for pristine chitosan. The mechanical properties of the films can be tuned from elastic (~ 8 MPa) chitosan films to stiff (~ 285 MPa) bionanocomposite films with 50% filler. The magnetic hyperthermia tests showed a temperature increase of 40 °C in 45 s from the 50% rGO-Fe₃-xO₄ film. Furthermore, the composites are cytocompatibles with HaCat cell lines.

Abstract ID: 694

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Composite structural materials

Keywords: Interface Layer, Insulating Property, SAXS

Temperature Dependence Interface Layer Structural Evolution of Composite Films by SAXS

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Polymer matrix dielectric is a newly composite material with rapid development, which is widely used in insulation of the electrical machinery and high voltage cable. Many scholars devoted to the study of the material, and put forward some theories of insulating property. The interface layer theory is the most attention and recognition. But, it is very difficult to test interface layer by conventional detection methods. In our work, the melt-blending process was adopted to prepare some Low-Density Poly-Ethylene composite films, to study the influence of the microstructure evolution of the composite film when the temperature changes. The results show that there are interface layers between nano-particles and polymer matrix in composite films. When 20 to 180 °C, the interfacial thickness increases from 2.8 to 3.5 nm, and remains constant beyond 100 °C. DSC shows that this increase is mainly caused by the melting of lamellae of polyethylene polymer chains. When temperature changes from 30 °C to 70 °C, the conductivity values of the composite film is significant different from pure LDPE. The conductivity of the composite film becomes two orders of magnitude smaller than that of pure film. The increases of interface layer limit the space charge accumulation effectively, and lowers the sensitiveness of conductivity to temperature, resulting in significant improvement of insulating property.

Abstract ID: 695

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Modeling and simulation of nanomaterials and predicting new nanomaterials and functional structures

Keywords: BNNTs, Enantioseparation, DFT study, Chiral drugs

Efficient performance of boron nitride nanotubes as chiral selector for separation of ibuprofen enantiomers using DFT-D3 calculations

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The separation of drug enantiomers in the pharmaceutical industry is of great importance since most organic compounds are chiral. In this study, we have evaluated the performance of chiral boron nitride nanotube (BNNT) for separation of ibuprofen enantiomers. The interaction between R- and S-isomers of ibuprofen with the outer surface and internal sidewall of chiral BNNT was investigated. The main purpose of this work is to calculate the binding energy of ibuprofen isomers interacting with the BNNT, according to various adsorption configurations. All calculations were performed by the DFT method with revPBE functional and GGA approximation. For this aim, the geometry of all interacting systems was optimized and energy calculations were performed by triple- ζ plus polarization basis set (def2 -TZVP). The long-range dispersion interactions have been considered by a combination of Grimme's atom pair-wise dispersion corrections with Becke–Johnson damping. The impact of the incomplete nature of the basis set in non-covalently bonded systems was attenuated using counterpoise correction to diminish the basis set superposition error (BSSE). The adsorption energy difference between R- and S-enantiomers inside the BNNT was about 0.62 kcal/mol, while this energy difference for adsorbed enantiomers onto the outer surface of the nanotube was about 1.25 kcal/mol. The results of this study showed that there is a significant difference between the adsorption energy of the enantiomers incorporated into the BNNTs, therefore we can anticipate this nanotube will work effectively in the process of separating drug enantiomers. In our previous study, the performance of carbon nanotubes (CNTs) as chiral selectors in the separation of ibuprofen isomers was investigated by similar calculation procedures. The energy difference between the pair of adsorbed enantiomers in the internal and outer sidewall of CNTs was about 0.2 and 0.0 kcal/mol respectively, indicating that BNNTs are more effective in the process of separating ibuprofen enantiomers rather than CNTs counterparts.

Abstract ID: 696

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Biomaterials for soft tissue applications

Keywords: Metallofullerenol, SAXS, Transferrin

Metallofullerenol Inhibits Cellular Iron Uptake By Specially Inducing Transferrin Tetramerization

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Herein, A549 tumor cell proliferation was confirmed to be dependent on the concentration of Fe³⁺ or transferrin (Tf). Gd@C₈₂(OH)₂₂ or C₆₀(OH)₂₂ effectively inhibited the iron uptake and the subsequent proliferation of A549 cells. The conformation changes of Tf mixed with FeCl₃, GdCl₃, C₆₀(OH)₂₂ or Gd@C₈₂(OH)₂₂ were obtained by SAXS. It is demonstrated that Tf homodimers were decomposed into monomers with FeCl₃, GdCl₃ or C₆₀(OH)₂₂, but aggregated into tetramers with Gd@C₈₂(OH)₂₂. The SAXS shape of Tf+C₆₀(OH)₂₂ had a larger change compared with Tf+FeCl₃, implying that C₆₀(OH)₂₂ bound to Tf to jam the iron binding site. The larger deviation of SAXS shape from a possible crystal structure of Tf tetramer implied that Gd@C₈₂(OH)₂₂ bound to Tf tetramer to disturb iron transport. This study well explains the inhibition mechanism of Gd@C₈₂(OH)₂₂ and C₆₀(OH)₂₂ on iron uptake and the proliferation of A549 tumor cells and highlights the specific interactions of nanomedicine with the target biomolecules in cancer therapy.

Abstract ID: 697 / Poster: 10

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Biomaterials for hard tissue applications

Keywords: Small Angle X-Ray Scattering, Protein Size

Measurement of Protein Size in Concentrated Solutions by Small Angle X-Ray Scattering

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The distance distribution function $P(r)$ of a dense system of monodisperse spheres, which may be obtained from the scattering intensity using the Fourier transform:

Where $I(q)$ is the scattering intensity, q is the scattering vector, $P(r)$ is related to the frequency of certain distances r within a particle. Therefore, it starts from zero at $r=r_1=0$ and goes to zero at $r=r_2=2R=D_{\max}$ (the maximum distance in the particle).

By simulations on the distance distribution function (DDF) derived from small angle X-ray scattering (SAXS) theoretical data of a dense monodisperse system, we found a quantitative mathematical correlation between the apparent size of a spherically symmetric (or nearly spherically symmetric) homogenous particle and the concentration of the solution.

Where K is a constant. Obviously, $\ln r^2$ versus $c^{0.52}$ presents a linear line, and D_{\max} can be derived from the linear line intercept.

Fitting the data in Figure 1 (a) and (b), it yields the maximum size D_{\max} values of human hemoglobin and horse myoglobin as 6.5nm and 4.7nm, which are close to the value of 6.4nm and 4.4nm available in literatures [1,2], respectively. These validated the correlation (2). This gives a new method to determine, from the DDF, the size of spherically symmetric (or nearly spherically symmetric) particles of a dense monodisperse system, specifically for protein solutions with interference effects.

Wednesday, 21/Aug/2019 5:24pm - 5:36pm

Abstract ID: 698 / FBB-2: 8

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Implant Development

Keywords: Indwelling Catheter, Antimicrobial, Vibration

A New Antimicrobial Method Against Indwelling Catheter-related Infection

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Bacterial biofilm infection is particularly common in the use of indwelling catheter. However, the use of antibiotics and antimicrobial materials cannot effectively prevent infection, and the indwelling catheter-related infection remains a serious problem. In view of catheter-associated urinary tract infection (CAUTI), a new antimicrobial method was proposed in this paper. We coupled the piezoelectric element to the outside of the catheter to provide a low-power excitation signal which can generate nano-level vibration on the surface of catheter. The vibration can impeding the colony aggregation and biofilm formation on the surface of the catheter. Furthermore, the model of adhesion force between bacterial and the surface of catheter was established focused on *Escherichia coli* (ATCC 25922), and the mechanical effect of surface vibration on bacteria was discussed. Finally, the effectiveness of the new antibacterial method was preliminarily proved by experiments. This study offers a new idea for the anti-infection method of indwelling catheter, and further development of the method can benefit the implanted medical device industry.

Abstract ID: 701 / Poster: 20

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Catalysis for Chemical Synthesis

Keywords: Metallo porphyrin, TiO₂, Rhodamine, Visible light, Photocatalysis, Photodegradation

Study on Visible Light Photo-Sensitized Metallo-Porphyrin/TiO₂ and its Photocatalytic Activities

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Young-A Son¹**

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Organic dye degrading property in Poly Ethylene Terephthalate polymer through photo catalytic effect by metallo porphyrin and TiO₂ has been studied in details. The surface has been modified by step wise deposition of anatase TiO₂ and metallo porphyrin, photocatalytic property of the modified fabric surface has been studied by photo degradation of zanthene dye by irradiation under visible light and the degrading ability and the efficiency has been monitored UV-Vis spectral technique by measuring the change in concentration of zanthene dye at different time intervals. Stability of metallo porphyrin also measured by UV-Vis spectral method indication the porphyrin attached in the sample surface are highly stable after washing the samples with detergent, water even after irradiating under visible light for more than 5h. The modification that is the deposition of TiO₂ and porphyrin made in the test samples were characterized and confirmed by XRD, XPS, UV-Vis, FESEM analysis and the prepared metallo porphyrin has been confirmed through mass analysis.

Abstract ID: 702

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: Key Words: DDM-containing epoxy resin; chromogen; ultraviolet light

The Chromogen, Structure, and Applications of a Photo , pH , thermal , Solvent-, and Mechanical-Response Epoxy Resin

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Epoxy resin has been widely used in many fields because of its good mechanical property. In some special fields, people need particular kinds of epoxy resin that is able to respond to the change of environmental conditions, especially if the color changes can indicate whether or not a part is in jeopardy of failing. However, epoxy resin is an ordinary structural material, which is normally unfunctional. Accidentally, we found the 'ordinary' DDM-containing epoxy resin framework turns the color from light brown to green gradually when it exposed to sunshine at room temperature. Considering that the raw materials in this epoxy resin framework do not contain any chromogen, the mechanism of this chromogenic phenomenon attracts our interests. Herein, we report the finding of a photochromic phenomenon from a structural epoxy resin, which is sensitive to the ultraviolet light in sunshine, and also has pH-, thermal-, solvent-, and mechanical-response property. Through designing model compounds and doing confirmatory experiments, we find out that one kind of diarylmethane dye (Michler's hydrol blue) is the chromogen of this epoxy resin. Additionally, we propose and successfully verify the mechanism of this novel color-change phenomenon that it is an oxidation-heterolysis mechanism. This discovery process is inspiring, which adds functional nature into the realm of 'ordinary' epoxy resins.

Abstract ID: 703

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: epoxy resin; phase change material; facile preparation

A reliable epoxy-based phase change material: facile preparation, tunable properties, and phase/microphase separation behavior

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Room-temperature-use phase change materials (PCMs) are of vital importance in combining the sustainable development of energy with human comfort. Here, a series of novel epoxy-based polymeric solid-solid PCMs (SSPCMs) were facilely prepared by UV grafting 1-octadecanethiol (ODT) onto an allyl-based epoxy resin (DADGEBA) via thiol-ene click chemistry followed by the epoxy-amine thermal curing process. Therefore, the grafted ODT can be tightly locked in a reliable three-dimensional crosslinking network of the epoxy resin, which provides the PCMs with excellent shape-stable property. Phase change and mechanical properties characterized by DSC, DMA, hardness test, and tensile test can be easily tuned by adjusting the mass ratio of DGEBA and the ODT-grafted-DADGEBA product (D18), which was characterized by FTIR and NMR. XRD and POM analyses proved the crystallinity of EPD18-X PCMs. The structure and morphology of the EPD18-X PCMs were characterized by visual images, SEM, and POM analyses. Microphase separation was observed in all the EPD18-X PCMs, and an obvious phase separation was observed in the EPD18-25 system. However, the phase separation gradually disappeared with the increasing of the D18 content. Thermal recycling tests showed that EPD18-X PCMs can remain stable after 50 DSC thermal cycles. Due to the unique strong encapsulated epoxy curing networks, EPD18-X PCMs have excellent thermal stability with the onset degradation temperature higher than 250 °C. Tunable EPD18-X systems can be applied for room-temperature-use thermal energy storage applications such as buildings, thermoregulated fabrics, and so on.

Abstract ID: 704

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Metal oxide, carbon, nitrides etc based thins Films

Keywords: Pulse reverse current, Microhardness, Wear, Microstructure, Composite coatings

Influence of pulse reverse current electroplating parameters of Ni - nano Al₂O₃ composite coatings on AISI 304 stainless steel

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Ni-nanoAl₂O₃ composite coatings studied by pulse reverse electroplating technique. AISI 304 stainless steel has been used for experimentation. Pulse reverse current parameters (PRC) of duty cycle, current density and frequency are identified as grain refining parameters. Besides the number of pulses played a vital role in obtaining perfect coatings and change of hardness is linear way. Lesser hardness is obtained in higher frequencies and higher hardness in lesser frequencies, certain change in their linearity shows the effect of number of pulses induced. Based on the above observations higher frequencies, number of pulses has been reduced, for lower frequencies numbers of pulses have been be increased. Obviously frequency has an inversely proportional relationship with numbers of pulses. The optimum PRC frequency (2 forward and 2 reverse ON + OFF time) of 175 Hz produced strong embedded nanoAl₂O₃ microstructure, 697.6 Hv and the wear rate of (2 kg) coating withstood for 160 seconds and 167.46 mm distance.

Abstract ID: 705

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

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

Keywords: 2D materials, DFT, CI-NEB, Solvation Model

Role of Electrolytic Solvents in 2D anode Based Batteries

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In general, for screening two-dimensional (2D) electrode materials, density functional theory (DFT) calculations are conducted without considering possible environmental effects arising from liquid electrolytes¹. Neglecting such effects could impact the accuracy of the predictions as the electrolytes affect operation of batteries through both chemical interactions with the electrodes and electrostatic effects. While explicitly incorporating the electrolyte molecules in DFT simulations is desirable, however, such computationally expensive investigations could be tedious if not impractical. In this work, we account for these dielectric effects using a quantum mechanics-based continuum solvation model wherein the electrolyte is incorporated as a polarizable continuous medium with a uniform dielectric constant, ϵ_r ². The electrostatic interactions between liquid electrolytes, solute Li atoms, and graphene, hexagonal boron nitride, or black or blue phosphorene were evaluated for a total of thirty electrolytes of differing ϵ_r . Our calculations show that for all the 2D materials investigated, the binding energy (EB) of Li on each substrate increased with rising dielectric constant relative to vacuum. This effect is missed when employing conventional DFT methods. However, with larger ϵ_r , EB for Li on graphene increases monotonically, whereas it reaches a plateau for black phosphorene and decreases in blue phosphorene above a value of 34 for ϵ_r . Electronic structure calculations revealed that for all the materials, for values of ϵ_r greater than 1, Li ions donate states at the Fermi level which increases the system's electronic conductivity. To assess the energy barriers (E_a) associated with the diffusion of Li atoms over the 2D substrates, we carried out Climbing Image Nudged Elastic Band simulations which indicated that with a rise in ϵ_r , the values of E_a decreases by orders of magnitude over all the substrates. These results suggest that the diffusivities predicted by standard DFT are orders of magnitude smaller than potentially observed values via proper electrolyte selection. Our results not only provide unprecedented insight into the interactions between 2D electrode materials, solute atoms, and the electrolytes, but also serve as a starting point for rational cell design.

Thursday, 22/Aug/2019 3:15pm - 3:30pm

Abstract ID: 706 / FCM-4: 7

Symposium 2: Functional Composite Materials (FCM)

Plenary

Topics: Composite structural materials

Keywords: Ti/Al₂O₃ composites; sintering aid; mechanical properties

Fabrication and mechanical properties of Ti/Al₂O₃ composites with CeO₂, Y₂O₃, and ZrO₂ doped

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Ti/Al₂O₃ composites doped with CeO₂, Y₂O₃, and ZrO₂ were successfully fabricated via pressureless sintering in Ar atmosphere at 1450 °C to discuss the reinforced effect of various sintering aids comparing with the blank materials. Thereinto, Ti/Al₂O₃-CeO₂ composites have been demonstrated being endowed the best mechanical properties with the porosity of 19.33%, bending strength of 178.26 ± 2.14 MPa, and fracture toughness of 2.53 ± 0.11 MPa•m^{1/2}, respectively, which was attributed to the contribution of tough phase CeAlO₃. Fracture toughness and bending strength have both increased upon 20% than these of Ti/Al₂O₃ composites. Meanwhile, the toughening mechanism has been studied via analyzing the microstructure and phase component.

Thursday, 22/Aug/2019 3:00pm - 3:12pm

Abstract ID: 707 / FTF-2: 6

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Organic and polymer film

Keywords: Mesophase Semiconductor, Self-assembly, Charge Carrier Mobility

Novel Pi-Electron Molecular Scaffolds for Mesophase Semiconductors

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Organic electronics is an exciting research field, attracting researchers from chemistry, physics, materials science and engineering. The fabrication of organic electronic devices including field-effect transistors, light-emitting diodes, and photovoltaic solar cells needs high performance polycyclic aromatic hydrocarbon materials. The molecular designing, synthesis, purification of novel pi-electron scaffolds is prerequisite for the development of organic electronics.

Mesophase semiconductors are self-assembled, dynamic, ordered, supramolecular electronic materials, displaying high ambipolar charge carrier mobility with featuring of electrical field and temperature independence, and defects self-healing ability.

In this presentation, we will report our works on discotic liquid crystalline donor-acceptor dyads and triads with segregated assembly for separated electron and hole pathways; effect of molecular conformation on mesophases, dynamics, and charge carrier mobility. The emphasis of this report will put on our novel molecular designing and facile synthesis of these pi-electron molecular materials, their self-assembled supramolecular structures.

Abstract ID: 708

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Sodium Ion Batteries

Keywords: Graphene, Sodium Ion, Energy Storage, SnS

Self-Assembled SnS Particles Electrostatically Anchored on Three Dimensional Dual Doped Holey Graphene for High Performance Sodium Ion Batteries

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Sodium ion batteries (SIBs) because of their low cost and reasonably good performance have gained importance for large scale energy storage systems. For these batteries to be commercialized, we require an anode material of having high capacity, high rate capability, and good cyclic stability. Among different anode materials, two-dimensional (2D) transition metal dichalcogenides (TMDs) have gained a lot of attention because of their good theoretical capacity. Layered tin(II) sulfide is one such material that exhibits a large theoretical specific capacity (1028mAh/g) however, low electronic conductivity, large volume changes during sodiation/desodiation decrease the capacity retention as the number of cycles are increased. Many approaches have been designed recently to counteract these problems and herein, by using a facile hydrothermal route. A possible pathway to cater these disadvantages is carried out by anchoring tin (II) sulfide nanostructure electrostatically through functionalization on three dimensional nitrogen sulfur co-doped holey graphene. It has already been observed that 3D architecture of graphene can provide enough space to cater volume expansion during sodiation/desodiation and its highly interconnected hierarchical, porous structure can improve electron transport and ion diffusion properties. This paper will analyze the impact on cyclic life, specific capacity and its degradation for as prepared composite when it is used as an anode material for sodium ion batteries.

Abstract ID: 709

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Electrochemical Supercapacitors

Keywords: Graphene, Hydrothermal, Metal Oxide, Nanocomposite, Supercapacitor

Charge storage behavior in flower structure of rGO-MnO₂ nanoparticles for supercapacitor application.

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Charge storage behavior in flower structure of rGO-MnO₂ nanoparticles for supercapacitor application

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Supercapacitors as a class of energy storage devices with high power density and long life cycle are of interest in a wide range of application from commercial product, electronics to hybrid vehicles and military devices. Nowadays most researchers have been focusing on the development of transition metal oxides due to their redox reaction. In this regards various types of the metal oxide and its composites were investigated. Among them, MnO₂ has been widely studied as the pseudocapactive electrode material of high-performance supercapacitors for its large operating voltage, low cost, and environmental friendliness. On other hand, the Graphene is a single atom thick, two dimensional sheet of sp²-hybridized carbon atoms arranged in a honeycomb crystal structure with exceptionally high strength, surface area, thermal conductivity, and electronic conductivity. Therefore an attempt was taken to develop a composite material which can meet the commercial requirement of storage devices.

In this regard, a simple hydrothermal process was used to design self-assembled MnO₂ nanoparticles are in porous flower structure in presence of graphene oxide (GO) as template. The reduced (rGO) offers not only a robust scaffold loading MnO₂ but also a conductive network for efficient ionic and electronic transport; thus, it is potentially promising as a novel electrode architecture for high-performance energy storage device. The structural analysis shows total four distinct reflection peaks of (001), (002), (111), (311) planes of δ -MnO₂. The microstructure images display the well defined porous flowers like structure of MnO₂nanoparticles with rGO. The FTIR shows Mn-O peaks at 448 cm⁻¹ and 515 cm⁻¹ in rGO-MnO₂ composites. Further, the Raman peaks of pure MnO₂ were observed at 332.02 cm⁻¹ and 640.47 cm⁻¹ whereas minor shifting of 2.65 cm⁻¹ and 1.96 cm⁻¹ in these peaks were observed respectively after GO addition. Charge storage capacity of pure MnO₂ and rGO-MnO₂ composite materials of different concentration of GO. The maximum specific capacitance value of rGO-MnO₂ composite of 463.94 F/gm was obtained for the rGO (25.42 wt%)-MnO₂.

Key words: Graphene, Hydrothermal, Metal Oxide, Nanocomposite, Supercapacitor.

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Thursday, 22/Aug/2019 11:24am - 11:36am

Abstract ID: 710 / FCM-3: 3

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Ceramic based composites

Keywords: Additive manufacturing, High performance ceramics, Porous structures

Effect of ceramic grain size on fabrication of porous ceramic parts using Solvent Based Slurry Stereolithography

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Additive manufacturing has gained a great attention over the last decade and many technological advances were made in terms of processes, materials, and applications. Solvent-based Slurry Stereolithography is a vat Photopolymerization process of fabricating high-density ceramic parts using high-performance ceramic materials like alumina, zirconia, etc. This process is capable of fabricating parts with up to 99.4% density for alumina with a flexural strength of 472 MPa and up to 98% density for zirconia with a flexural strength of 731 MPa. Although these characteristics are very helpful in applications like orthodontics, prosthetic implants, etc., such highly dense parts are not useful for applications like liquid infiltration, thermal insulators, catalyst supports, etc., where the workpieces need to have open channels, open dead-end pores, or closed pores. In this paper, the materials used in the slurry are exploited in depth to fabricate porous ceramic objects that can be useful for the infiltration applications. An in-depth investigation is carried out about the solvent content, granular size of the structure material, effects of addition of composites, and sintering parameters, to identify the best suitable combinations to fabricate various porous structures. The fabricated workpieces are then characterized by calculating the porosity, surface roughness, shrinkage rate, and flexural strength.

Abstract ID: 711

Symposium 2: Functional Composite Materials (FCM)

Invited Talk

Topics: Nanocomposites

Keywords: SERS, Langmuir-Blodgett, Liquid Crystal, PMMA, 4-MPy

Fabrication of SERS active substrates with Langmuir-Blodgett deposition technique

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Surface-enhanced Raman scattering (SERS) spectroscopy has been established as a powerful technique that allows enormous enhancement of Raman signals from probe molecules upon their adsorption on the nano structured surfaces. However, the remarkable analytical sensitivity of SERS has yet to be translated into the development of widely accepted, commercially viable diagnostic applications mainly because of the difficulty in preparing robust and correct surface morphologies that provide maximum SERS enhancements. In the present lecture, I share our recent experimental results leading towards fabrications of large area SERS active substrates through coherent integration of Langmuir-Blodgett (LB) and self-assembly technique. Highly reproducible and robust SERS active Neplas (Nematogens + Plasmonic materials) of type I and II substrates have been prepared from Langmuir Reverse Schaefer ((L-R Sh) films of 5-CB nematic liquid crystal molecules immersed in gold nanocolloids for 36 and 48 hours respectively.

Another kind of substrates of the monolayer LB film of PMMA molecule lifted at surface pressures 40 mN/ m and 10 mN/ m followed by incubation in gold nanocolloids for 24 hours. The plasmonic architectures of the substrates can be tuned to control the hot spots for the overall enhancements of SERS signal. These substrates are unique in their kinds, where explicit or concomitant presence of protonated and deprotonated forms of 4-MPy can be detected at trace concentrations. So, finally it can be concluded that these techniques are expected to provide new direction towards successful fabrication of next modern SERS sensing platforms

Abstract ID: 712

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Nanocomposites

Keywords: SERS, Hurst Exponent, Lateral Correlation Length, Lyapunov Exponent, Chaos

Self-affine properties of SERS active substrates: Experimental vis-à-vis theoretical investigations

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A facile fabrication of SERS active substrate by coherent integration of self assembly and Langmuir- Blodgett (LB) deposition technique has been reported. Enormous enhancement factor $\sim 10^{10}$ orders of magnitude have been estimated at trace concentrations of 4-MPy for the as prepared substrates. Moreover, in order to encounter the reason behind the high enhancement factor ($\sim 10^{10}$ orders of magnitude), some hidden parameters related to the topographical features that liable to the responses of the enhanced vibrational signatures of the molecule has been envisaged. The surface morphology of the as prepared substrates has been examined from the statistical concern like lateral correlation length (ξ), Hurst exponent (α), Lyapunov exponent (λ) in real space and from the power spectra in the reciprocal space. The real space of the substrates is taken from the AFM images of the as prepared substrates.

The AFM images of the substrates, thus captured are analysed from height- height correlation function $H(r)$, for various position of r on the surface. Figure 1 shows the variation of $\log H(r)$ as a function of $\log r$. Here exponent value ($\alpha \sim 0.7$), signify long range correlations ($\xi \sim 117- 155$ nm) driven by the superdiffusion of Au nanocolloids on the monolayer LB film matrix of PMMA. Interestingly ξ value sustain quite longer for the substrate lifted at 40 SP (Class “A” substrate) than 10 SP (Class “B” substrate). This may state the closely packed behaviour of PMMA molecule lifted at higher pressure helps nanocolloids more to get anchored with template and sustain height correlation longer length scale. The specific patterns of the as prepared substrates may be explained from the interplay of forces between long range nanoparticle- nanoparticle repulsion (FNMR) and short range forces arising from nanoparticle- nanoparticle attraction (FNNA), nanoparticle - monolayer lipophilic attraction (FNMA) and the monolayer - monolayer lipophilic attraction (FMMA). Among them, in our case, the force due to FMMA, arising from the monolayer LB films of PMMA is more effective for the substrate of class “A” lifted at higher pressure due to close alignment of molecules on the substrate. This also led FNNA & FNMA more effective to control the aggregation state between nanoparticles entrapped in LB film of PMMA driven by super diffusion process than lower surface pressure. Thus the FNNA and FNMA together may play a dominant role towards the generation of chaotic fractal patterns in the as prepared substrates.

Thursday, 22/Aug/2019 2:00pm - 2:12pm

Abstract ID: 713 / FTF-2: 1

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Optical, electrical and magnetic properties of thin films

Keywords: Transparent conductive thin films, electromagnetic interference (EMI) shielding, indium tin oxide, gold, magnetron sputtering.

Transparent and Conductive ITO/Au/ITO Multilayer Thin Films with Enhanced EMI Shielding Properties

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Highly transparent and conductive ITO/Au/ITO multilayer coatings were deposited onto the soda lime glass (SLG) via magnetron sputtering without substrate heating. The thicknesses of each ITO and Au layers of the films were optimized to improve the overall transparency and conductivity of the coatings by adjusting the Au and ITO deposition times, respectively. As-prepared thin films were characterized by many techniques, including X-Ray Diffraction, Scanning Electron Microscopy, Transmission Electron Microscopy and Atomic Force Microscopy. The optical measurement results revealed that the transmittance of the films were enhanced by increasing the duration of gold deposition up to a limit of 15 seconds. Beyond this limit, further increasing the gold deposition duration resulted in the loss of the optical transmittance. Upon optimization of the Au deposition time, the highest transparency value of 82.7 % at 550 nm was reached within the sample showing the electrical conductivity of 3551 S/cm. Then, using the best Au deposition duration, the thicknesses of the ITO layers in the films were also optimized. Accordingly, the highest transparency of the films was reached at 84.2 % with the electrical conductivity of 4159 S/cm. Following to this, the films were deposited onto a polymer substrate to converge industrial application. The EMI shielding performance of these ITO/Au/ITO films on the polymer substrates were studied. Finally, we propose here a new multilayer thin film design that provided enhanced EMI shielding performance, as evidenced by corresponding tests.

Abstract ID: 714

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nanomaterials for Sensors, Flexible Electronics and Nanocomposites

Keywords: Silicon, Nanowire, detectors, plasmon, hybrid nano structures

Functional Nanowires for Device Applications; Electronic Plasmonic-enhanced Near-Infrared Detectors Using Nano-Floret Hybrids

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We recently demonstrated the synthesis of a new class of hybrid nanostructures termed "Nano-Florets". The semiconductor-metal hybrid nanostructures resemble the morphology of grass flowers, consisting of a high aspect ratio SiGe nanowire (NW) with a metallic nanoshell cap. We demonstrate the fabrication of self-forming nanogap junction devices taking advantage of the unique structural motifs of the nano-florets. We demonstrate a simple method for device fabrication without the need for high resolution lithography enabling electronic measurements across molecules and nanoparticles. Connecting the NF nanojunction to the micro-, and macro-scales is achieved by applying standard, robust, optical lithography. In addition, the devices are operable at ambient conditions and in various solvent environments. Furthermore, introduction of quantum dots results in the mapping of their band structure at ambient conditions. The metallic tip of the hybrid nanostructures show plasmonic absorption extend to the NIR and to the short wave infrared (SWIR) spectral ranges. we present device concept for NIR-SWIR detection using these hybrid nanostructures. Plasmonic gain of three orders of magnitude is obtained with improved time response compared to nanowire-based detector due to the metal-semiconductor Schottky junction. Our results provide a proof-of-concept of large scale self-forming nanogap device platform realized using simple fabrication tools. Such a technology can be used for molecular detectors, as a potential building block for molecular electronics, or as a platform for fundamental research.

Abstract ID: 715

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Organic and polymer film

Keywords: graphite phase carbon nitride, membrane, permeation, enantioselectivity

Graphite phase carbon nitride based membrane for achiral/chiral separation

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Membrane separation featured with easy operation, green and low-cost is promising technic in many applications.1-2 Organic polymers are easy to form membranes of high quality, however, it is hard to control the pore size distribution in polymer membrane. In contrast, crystalline materials having narrow and definitive pore size and structure are difficult to form ideal membrane as presence of crystallite boundary. Advance on graphene oxide (GO) membrane has proven that two-dimensional materials are ideal candidate for membrane fabrication and the interlayer spacing can be controlled at molecular precision via intercalation of water layers, cations and nanomaterials into GO sheets for permeation study. However, most applications of current GO membranes are limited to water purification and water desalination, etc. The specified tasks like enantioselective separation in pharmacy industry calls for chiral membranes applicable in varied solvents.

Graphite phase carbon nitride (GCN), considered as a nitrogen-substituted graphene-like two-dimensional carbon material, is facile to be delaminated into single layers for membrane assembly. In comparison to GO with uneven and random distribution of oxygenous groups, the lone-pair electron on proportioned sp² nitrogen makes GCN apt to be protonated and soluble in strong acidic medium. In this work, we demonstrate the anion intercalation into protonated GCN sheets to tune not only the interlayer spacing but also the chemical environment (i.e., chirality) of the interlayer space for achiral/chiral separation in aqueous/organic solution.

Abstract ID: 716

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Nanomaterials for Photonics and Optoelectronics

Keywords: Hybrid Perovskite, Layered Structure, Photodetector

Controlling the Crystallization Process in Hybrid Perovskite Films for Photodetector Application

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The organic-inorganic perovskite materials have recently attracted broad research interests for their promising optoelectronic applications including photodetectors.¹ Compared with the ABX₃ three-dimensional structure, the reduced-dimensional perovskite, where the bulky organic cation A separates the framework [BX₄]₂⁻ into the layered structure A₂BX₄, shows superior environmental stability and tunable semiconductor properties according to its artificial quantum well structure. Moreover, the band gap of layered perovskites changes continuously depending on the number of [BX₄]₂⁻ layers n between the layers of organic cation A. Here we present that the crystallization process of reduced-dimensional perovskites can be controlled by anti-solvent treatment during the spin-casting fabrication, which facilitates the formation of a pure n=2 phase in the obtained thin films. In addition, we show that the hot-casting preparation of n=1 perovskite can create abundant below-gap states and increase the density of charge carriers for charge transport. Our findings are beneficial for the fabrication of high-quality hybrid perovskite films for high-performance photodetectors.

Wednesday, 21/Aug/2019 5:15pm - 5:27pm

Abstract ID: 717 / FC: 7

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalysis for pollution control

Keywords: Visible light photocatalysis, Carbon quantum dots (CDs), Ti³⁺ and nitrogen co-doped TiO₂, CDs-N-TiO_{2-x}, photoreduction of Cr(VI)

Facial fabrication of carbon quantum dots (CDs)-modified N-TiO_{2-x} nanocomposite for the efficient photoreduction of Cr(VI) under visible light

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Due to the wide use of hexavalent chromium (Cr(VI)) in metal finishing, steel fabrication and other industries, the difficulty posed by Cr(VI)-containing wastewater has become the focus of industrial wastewater treatment. Among the numerous technologies, the photocatalytic process, especially visible light photoreduction of Cr(VI), has attracted extensive research interest, due to its low cost, excellent performance, and the potential sustainability of green solar energy. In this study, a novel CDs-N-TiO_{2-x} nanocomposite was successfully fabricated by decorating the carbon quantum dots (CDs) on the nitrogen (N) and Ti³⁺ co-doped TiO₂ nanoparticles using a facile hydrothermal-calcination method. The crystal structure, morphology, optical property, and chemical composition of the CDs-N-TiO_{2-x} nanocomposite were investigated via several characterizations. Owing to the synergy between the modification of CDs and co-doping of N and Ti³⁺, the as-prepared CDs-N-TiO_{2-x} nanocomposite exhibited enhanced visible light absorption and more efficient charge separation compared with its counterparts, such as the pristine TiO₂, N-doped TiO₂ (N-TiO₂), N and Ti³⁺ codoped TiO₂ (N-TiO_{2-x}), and carbon quantum dots-TiO₂ (CDs-TiO₂), etc. As a result, the CDs-N-TiO_{2-x} nanocomposite displayed a remarkable performance for Cr(VI) reduction under visible light irradiation. Moreover, adding the appropriate amount of citric acid as the hole scavenger significantly increased the reduction rate of Cr(VI). In addition, the reduction efficiency was better under acidic conditions and considerably affected by the initial Cr(VI) concentration and catalyst dosage. Thermogravimetric analysis and cyclic runs demonstrated a unique thermal and chemical stability of the CDs-N-TiO_{2-x} nanocomposite. The mechanism of the enhanced photoreduction of Cr(VI) by the CDs-N-TiO_{2-x} nanocomposite was discussed based on all the characterization and experimental results. Moreover, the developed CDs-N-TiO_{2-x} nanocomposite also exhibited efficient photocatalytic performance to reduce the Cr(VI) contained in real laboratory wastewater. Findings of the present study highlight the great potential of CDs-N-TiO_{2-x} for the treatment of Cr(VI)-containing wastewater.

Abstract ID: 718**Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)****Oral Presentation***Topics:* Carbon Nanomaterials*Keywords:* Carbon nanotube, Yarn, Electrical conductivity, Doping, Annealing**Drastic improvement of CNT yarn electrical conductivity by chemical doping and annealing treatment****Yoann DINI^{1,2,3}, Jérôme FAURE-VINCENT^{1,3}, Jean DIJON^{1,2}**¹Univ. Grenoble Alpes, F-38000 Grenoble, France; ²CEA, LITEN ,DTNM, SCSF, LCH F-38054; ³CEA, INAC, SYMMES, STEP F-38054 Grenoble, France; yoann.dini@cea.fr

In electrical wiring, metal substitution by high conductivity materials like carbon nanotubes (CNT) is a near future challenge for high-end textile¹, aeronautic and aerospace applications². Several techniques exist to make CNT yarns. The most suitable, eco-friendly process for large-scale production is to directly dry spin CNTs grown by fixed- or floating-catalyst Chemical Vapor Deposition (CVD). However, CNT yarn conductivities have not yet reached that of copper. Our work aims to overcome the 1.0 mΩ.cm resistivity limitation faced by all CNT yarns spun from CNT arrays in the literature. In our previous work³, we found that, at room temperature, the electrical conductivity of the CNT yarn spun from CNT arrays is limited by the intrinsic conductivity of the CNTs and we insisted on the crucial need to increase the CNT structural quality. We will present our last work where we significantly increase the CNT yarn conductivity by doping and annealing treatments.

At CEA Grenoble, we developed a new p-type dopant for carbon nanotubes and graphene: platinum chloride IV (Patent: US20180142346). It shows very good performances in term of conductivity improvement, temperature stability and long term time stability. Our dopant improves the CNT yarn and web electrical transport. The resistivity is considerably decreased by a factor of almost 3 and the stability in room condition is excellent. The doped CNT web resistivity only increases by 15 % in 192 days. The very long term time stability of the platinum chloride makes it a very promising dopant for industrial applications.

The CNT structural quality is increased by annealing our CNT yarn at temperature between 2000 °C and 2500 °C and for durations up to 72 h⁴. We observe a large improvement in the CNT structural quality as shown by the Raman G/D ratio which increases from 1.6 for a pristine yarn to 15 for an 11 hours annealing time at 2250 °C. We find that the CNT resistivity decreases with the increase of G/D ratio i.e. with the increase of the CNT structural quality. The CNT yarn resistivity is clearly improved by the annealing at very high temperature: it decreases by a factor of 2, going from 1.6 mΩ.cm to 0.76 mΩ.cm. This low resistivity value (0.76 mΩ.cm) is the new world record for undoped CNT yarn spun from arrays (usually limited between 1 and 3 mΩ.cm).

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Abstract ID: 719

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Nanocomposites

Keywords: Electrodeposition, Ni-B-Cu, surface coating, corrosion, Nanomechanical

Electrodeposition of Cu on Ni-B nanocomposites improves its mechanical properties

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Electrodeposition of Cu on Ni-B nanocomposites improves its mechanical properties

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Abstract:

Surface coatings are of global importance because of their countless applications endeavoured by them. The coatings form a protective covering for materials against the vigorous types of mechanical agitation and erosion due to the corrosive solvents and environment impacts. The innovative efforts lead to the invention of new materials with fine quality and improvement of properties in the existing materials. Among many materials, preparation of Ni based binary/ternary composites has received considerable attention in recent years to improve their characteristics such as hardness, anticorrosive properties and wear resistance for wider industrial applications.

The present investigation was carried out to embed the Cu particles into matrices of Ni-B alloy in order to improve the coating hard-ness, morphological texture as well as to pre-vent corrective effects of aggressive and harsh media. The technique of surface coatings was performed by conventional electrodeposition method using dimethylamine borane (DMAB) as well as boric acid as reducing agent and complexing agent respectively. XRD results obtained showed that Ni-B coatings were initially amorphous in nature however, the in-corporation of copper to Ni-B lead to development of crystalline coatings. The surface morphology of the Ni-B nanocomposite coating is observed to be compact and consists of globular clusters of grains, whereas in case of the Ni-B-Cu alloy composite coating it is observed to be porous, rough and consists of crystals of different shapes. Later, the depo-sition of Cu tremendously increased the roughness of the Ni-B matrix. Furthermore, hardness test and potentiodynamic linear polarization technique confirmed that mechanical properties and corrosion resistance was enhanced significantly by addition of Cu in Ni-B coatings.

Key Words: Electrodeposition, Ni-B-Cu, surface coating, corrosion, Nanomechanical

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Thursday, 22/Aug/2019 8:12am - 8:24am

Abstract ID: 720 / FLNM: 2

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Novel 3D functional architectures consisting of low-dimensional nanomaterials

Keywords: 2D zeolites, catalysis, layered composites, drug delivery

Zeolites as low-dimensional materials combining nanopores and nanolayers

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Zeolites are one of the most valuable and useful commercial materials with exceptional catalytic and sorption properties arising from their microporous 3-dimensional framework structures. Surprisingly they were also found to produce nanometer thick layers as building units for the frameworks but can also be manipulated like the conventional 2D solids.^{1,2} As the latter, zeolites have been found to produce much greater variety of layered structures, close to 20 different types, than the conventional layered solids and in addition offered layers with inherent catalytic activity and possibly porosity in and across.³ The presentation will provide an update on classification of layered zeolites, which includes both different types of layered structures and frameworks affording layered forms (approximately 20). Then, I will present the recent breakthrough in producing colloid suspension of zeolite MWW mono-layers, which has significant fundamental implications and practical potential for producing various structures and composites. The mono-layers were confirmed by physical characterization including AFM and TEM microscopic studies and chemical methods entailing coagulation by combination with suitable agents. The mono-layer suspensions of zeolite MWW were used to prepare delaminated catalysts with high surface area and pore volume, and drug carries for controlled release studies. Liquid exfoliation⁴ of layered zeolites can be of interest in many practical areas and presents intriguing fundamental questions concerning aggregation, surface chemistry and transport through the layers. They can also be considered for fabrication of membranes.

Key Words: 2D zeolites, catalysis, layered composites.

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Abstract ID: 721**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Household and large-scale energy storage systems

Keywords: Phase Change Materials, Nanoencapsulation, Nanomagnetite, Graphite, Thermal Energy Storage

Advanced Phase Change Materials for Thermal Energy Storage and Management**Halime O. Paksoy**

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Phase change materials (PCM) possess high thermal energy storage capacities that can be utilized isothermally. Latent heat that accompanies phase change can be stored for later use and for controlling temperature. Recent material research on advanced PCMs look for answers to these 5 questions: 1-What kind of a container is suitable? 2-How compatible is this material with other components of the system? 3-How fast is the PCM's response? 4-How long can the material be exploited? 5-Is it sustainable / recyclable or both? Recent trends in PCM research to address these challenges are concentrating on developing new PCM composites and micro/nano encapsulation of PCMs. This paper presents three different applications of advanced PCMs recently developed by our Çukurova University(CU) thermal energy storage group. Nano-magnetite paraffin composite (1) was developed for the thermal management of Li-ion batteries. This requires very fast heat dissipation to prevent overheating that leads to thermal runaway. Thermal conductivity of paraffin used as PCM was increased by 48% after adding 10% nano-magnetite. Using the composite with a Li-ion 32V battery pack has kept temperatures within the required safe range of 20-55°C. CU 's the second advanced PCM was a fatty acid mixture, microencapsulated in a poly-methyl methacrylate-co-2-hydroxyethylmethyl acrylate shell structure. This caused the microencapsulated fatty acid to become compatible for mixing into concrete. This developed material was tested in prefabricated wall panels for passive solar energy use in our test building. Two years of monitoring of the test building showed 13% energy savings is possible with 10% addition to concrete mix. The last and 3rd application was for the recovery of waste heat in a dishwasher to increase its energy efficiency. Here, waste heat of used water from the first washing cycle was recovered by a graphite-enhanced paraffin. This stored heat was transferred to the incoming second washing cycle during the preheating of water. This application required less heating power during the second wash cycle, and also increased energy efficiency of dishwasher by 11%.

Key Words: Phase Change Materials, Nanoencapsulation, Nanomagnetite, Graphite, Thermal Energy Storage

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Thursday, 22/Aug/2019 8:36am - 8:48am

Abstract ID: 722 / FLNM: 4

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Applications of low dimensional, nano and 2D materials

Keywords: Multiwall Nanotubes, Adsorbed Superfluid Helium, Film Compressibility

Superfluid Onset and Compressibility of 4He Films Adsorbed on Multiwall Carbon Nanotubes

Gary A. Williams, Emin Menachekanian, Vito Iaia, Mingyu Fan, Jingjing Chen, Chaowei Hu, Ved Mittal, Gengming Liu, Raul Reyes, Fufang Wen

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Third sound measurements of superfluid 4He thin films adsorbed on 10 ± 1 nm diameter multiwall carbon nanotubes are used to probe the superfluid onset temperature as a function of the film thickness, and to study the temperature dependence of the film compressibility. The nanotubes provide a highly ordered carbon surface, with layer-by-layer growth of the adsorbed film as shown by oscillation peaks in the third sound velocity (Fig.1) at the completion of the third, fourth, and fifth atomic layers, arising from oscillations in the compressibility. In temperature sweeps the third sound velocity at very low temperatures is found to be linear with temperature, but oscillating between positive and negative slope depending on the film thickness. Analysis shows that this can be attributed to a linearly decreasing compressibility of the film with temperature that appears to hold even near zero temperature. The superfluid onset temperature is found to be linear in the film thickness, as predicted by the Kosterlitz-Thouless theory, but the slope is anomalous, a factor of three smaller than the predicted universal value.

Thursday, 22/Aug/2019 10:24am - 10:36am

Abstract ID: 723 / FLNM: 13

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Applications of low dimensional, nano and 2D materials

Keywords: Graphene oxide membrane, Conical nanopore, Ionic current rectification

Selectively enhanced ion transport in graphene oxide membrane/PET conical nanopore system

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Graphene oxide (GO) has become a promising 2D material in many areas, such as gas separation, seawater desalination, antibacterial materials and so on due to its abundant oxygen-containing functional groups and excellent dispersibility in various solvents. The graphene oxide membrane (GOM), a laminar and channel-rich structure assembled by stacked GO nanosheets, served as a kind of precise and ultrafast separation material has attracted widespread attention in membrane separation field. In order to break the trade-off between ion permeability and ion selectivity of separation membrane based on GOM, GOM/conical nanopore system is obtained by spin-coating ultrathin GOM on PET conical nanopore which possesses ion rectification property. Comparing to pure PET conical nanopore, the existence of GOM not only enhances the cation conductance but also makes the ion rectification ratio increase from 4.6 to 238.0 in KCl solution. Assisted by COMSOL simulation, it is proved that the GOM can absorb large amount of cations and act as cation source to improve the ion selectivity and rectification effect of GOM/conical nanopore system. Finally, the chemical stability of GOM/conical nanopore is also investigated and the corresponding results reveal that the GOM/conical nanopore system can perform the ion rectification behavior in a wider pH range than pure PET conical nanopore. The presented findings demonstrate the great potential applications of GOM/conical nanopore system in ionic logic circuits and sensor systems.

Abstract ID: 724

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Innovative Methods for the Structural Characterization of Thin films

Keywords: indirect band gap to direct band gap transition; strain; band bow

Modulation of the Electronic Structure of Ge_{1-x}Sn_x alloy films by Strain and Composition

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Direct band gap semiconductors are of more efficient optoelectronic properties and of alluring applications in industry. Group IV element/alloy semiconductors are Optical transitions of Ge_{1-x}Sn_x/Ge films on Ge substrate are characterized by high resolution X-ray diffraction, spectroscopic ellipsometry (SE) and Raman spectroscopy. Results show that transition energies dependence of composition appears the nonlinear behavior. The behavior can be indicated by the bowing parameters b . The influence of tensile strain on the nonlinear behavior may be identified by the bowing parameters ratio. The strain structure has great impact on the bowing parameters. Moreover, the effect of the tensile strain on the direct bandgap energies and indirect bandgap energies is negative. And the deference of decreased direct and indirect band gap energies for tensile strained GeSn films is larger than that for relaxed GeSn films. That is responsible for the higher Sn composition when the indirect band gap changes to direct band gap for strained GeSn films. The transition from indirect band gap semiconductor to direct one in the present is determined to be $x=0.105$ at 300K.

Abstract ID: 725

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Solar Cells

Keywords: Dicationic imidazolium, Organic ionic plastic crystals (OIPCs), DSSCs, Solid-state electrolyte

Dicationic Imidazolium Iodide Plastic Crystals for a Solid-State Electrolyte of Dye-Sensitized Solar Cells

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A series of dicationic imidazolium diiodide salts is discovered as a new organic ionic plastic crystal. The feature of the new imidazolium salts is their multiple solid-solid phase transitions below their melting temperatures. All solid-solid transitions and melting points are dependent on the chemical structure of the dicationic imidazolium cations. Bis-imidazolium diiodides with either n-heptyl (C7) or n-octyl (C8) side arms can be classified as “true plastic crystals” by Timmerman’s definition of plastic crystals: low ΔS_f values. $< 20 \text{ J mol}^{-1} \text{ K}^{-1}$. The most prepared imidazolium iodide salts are stable up to 260 °C under N₂ from thermal gravimetric analysis. The ionic conductivities follow the Arrhenius temperature dependence with discontinuities and changes in slopes at their solid–solid phase transition temperatures. Using n-hexyl side-armed bis-imidazolium iodide (BII-6), dye-sensitized solar cells (DSSCs) fabricated by a whole solid-state electrolyte show a 4.93% power conversion efficiency (η), which is a notable result for the whole solid-state electrolyte. For comparison, DSSCs using a liquid electrolyte with 1-butyl-3-methylimidazolium iodide shows $\eta = 8.00\%$ as a reference composition.

Thursday, 22/Aug/2019 9:00am - 9:12am

Abstract ID: 726 / FESC: 6

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Nanostructured materials for advanced batteries

Keywords: Graphene; TiN Nanowire; Shuttle Effect

Three-Dimensional Nitrogen-Doped Graphene/TiN Nanowire Composite as a Strong Polysulfide Anchor for Lithium-Sulfur Batteries

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Lithium-sulfur (Li-S) batteries have attracted remarkable attention due to their high theoretical capacity of 1675 mAh g⁻¹, rich resources, inexpensiveness, and environmental friendliness. However, the practical application of Li-S battery is hindered by the shuttling of soluble lithium polysulfides and slow redox reactions. Herein, we report a three-dimensional nitrogen-doped graphene/titanium nitride nanowires composite (3DNG/TiN) as a freestanding electrode for Li-S battery (Figure 1). The highly porous conductive graphene network provides efficient pathways for both electrons and ions. TiN nanowires attached on the graphene sheets have strong chemical anchor effect on the polysulfides, which is proved by the superior performance and density functional theory calculations. As a result, the 3DNG/TiN cathode exhibits an initial capacity of 1510 mAh g⁻¹ and the capacity remains 1267 mAh g⁻¹ after 100 cycles at 0.5 C. Even at 5 C, a capacity of 676 mAh g⁻¹ is reached. With a high sulfur loading of 9.6 mg cm⁻², 3DNG cathode achieves an ultra-high areal capacity of 12.0 mAh cm⁻² at the high current density of 8.03 mA cm⁻². This proposal unique structure gives the bright prospect that high energy density and high power density can be achieved simultaneously for Li-S battery.

Abstract ID: 727

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Magnetic film

Keywords: transport properties; YBa₂Cu₃O₇/LaCaMnO₃ bilayers; superconductivity; magnetic properties

Transport properties in YBa_{1.85}Eu_{0.15}Cu₃O_{7-δ}/La_{0.67}Ca_{0.33}MnO₃ superlattices grown on (001) SrTiO₃ substrate

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High quality YBa_{1.85}Eu_{0.15}Cu₃O_{7-δ}/La_{0.67}Ca_{0.33}MnO₃ superlattices with varying the thickness of the sublayer are grown on (001) SrTiO₃ (STO) substrate by magnetron sputtering technique. All films show well c-orientation and four-fold symmetry. Strain of the films is characterized. Transport properties measurements reveal that the superconductivity and ferromagnetism coexist but compete in the films depending on the growing sequence and the thickness of each sublayer. In the superlattice of (YBECO₂₇ nm/LCMO₆nm)₆, we not only observe the coexistence of superconductivity and ferromagnetism for magnetic field H parallel (H || ab) to substrate, but also observe the magnetization oscillation behavior near H = 0 for H perpendicular (H || c) to the substrate. We attribute this oscillation with the surface flux pinning.

Abstract ID: 728

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Industrial applications of composite materials

Keywords: nanoparticles, transparent dispersion, large-scale production

Mono-dispersed Nanoparticle and Its Functional Optical Nanocomposite

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How to disperse the inorganic nanomaterials mono-uniformly in the organic matrices is the key challenge of innovation of new generation of organic-inorganic nanocomposites. Many techniques have been used to fabricate the transparent nanocomposites by incorporating the mono-dispersed nanoparticles into optical polymer. However, making mono-dispersed nanoparticles requires complex processing, and it is difficult to realize large-scale production. In this paper, a simple strategic method to synthesize the mono-dispersed nanoparticles in the liquid mediums (transparent nanodispersions) was proposed to prepare the transparent polymer-based nanocomposites. The transparent nanodispersions with the contents higher than 50 wt% were produced by our proposed novel high-gravity reaction coupled with extraction-phase transfer (HGRT) technology. By such strategy, the various transparent nanodispersions and their polymer-based nanocomposites with unique functions were fabricated on a large-scale, such as metal oxides nanodispersions, nano-lubrications for high railways and nanocomposite films for glass energy-saving, where the inorganic nanoparticles were all dispersed at the nano-scale. Even if the content of nanoparticles was higher than 50 wt%, the fabricated flexible nanocomposite film also had the same visible transmittance with the unfilled film. Our HGRT technology is suitable for massive production of transparent nanodispersions and functional optical nanocomposites, which is cost effective and the products for the custom designed nanoparticles for tailored functions.

Abstract ID: 729

Symposium 2: Functional Composite Materials (FCM)

Invited Talk

Topics: Composite structural materials

Keywords: Meta-atom, SAR, SRR

Electromagnetic Absorption of SRR Based EF-Structured Meta-Atom for DCS, EESC, 5G, and WiMAX Applications

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In this article, a novel split ring resonator (SRR) loaded EF-structured meta-atom is presented, proposed, and investigated for digital cellular system (DCS) (1820 MHz), earth exploration-satellite (2220 MHz) communications, lower band 5G mobile (4820 MHz) communications, and WiMAX (5920 MHz) applications. Furthermore, the meta-atom is also utilized to investigate its electromagnetic (EM) absorption reduction performances at above mentioned frequencies. Finite-difference time-domain method based Computer Simulation Technology Microwave Studio software has been utilized for the design and brief analysis of the meta-atom. The introduced meta-atom has been formed by developing EF-structure in addition with SRR which is embedded on Flame Retardant-4 (FR4) dielectric substrate and the size of the meta-atom is 11.12×11.12 mm², which is shown in Figure 1. The meta-atom has a high effective medium ratio of about 14.82. The meta-atom also exhibits double-negative characteristics over the frequency ranges from 3.94–4.57 GHz, 5.26–5.49 GHz, 6.29–6.88 GHz and negative refractive index from 3.124–7 GHz. Moreover, SAR evaluation also has been done to check the compatibility of using it on the modern handset devices [1]. The meta-atom has electromagnetic absorption rate about 84% and 78% at 1800 MHz and 2220 MHz, respectively for 1gm whereas it has reduction rate about 91% and 90% at 1800 MHz and 2220 MHz, respectively for 10gm.

Overall, a novel meta-atom has been presented where the compactness of the size of the meta-atom and its performances makes it compatible to use for the applications of 1820 MHz, 2220 MHz, 4820 MHz, and 5920 MHz, respectively.

Abstract ID: 730

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin Films in Biological and environmental Applications

Keywords: Key Words: Activated Carbon, Coating, Methylene Blue, Adsorption, HDPE.

Investigation of Activated Carbon Coating in the Adsorption Process of Methylene Blue from Aqueous Solution

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Investigation of Activated Carbon Coating in the Adsorption Process of Methylene Blue from Aqueous Solution

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This research evaluates various coating methods and conditions of granular activated carbon (GAC) on high-density polypropylene (HDPE) in the attempt to use coated HDPE for adsorption applications. Four HDPE substrates were coated by using either sol-gel method, namely TEO, or Paint-Spray-Dry method, namely applying epoxy resin to HDPE using brushing technique and spraying the AC on the epoxy layer. The ability of these coated surfaces to remove methylene blue (MB) were then investigated. In addition, the durability of the coatings was characterized by using Energy Dispersive X-ray (EDX) and Scanning Electron Microscopy (SEM) on Day 1 and Day 28. Results show that the activated carbon demonstrated a good adsorption capacity of 12.75 mg/g at 50 mg/L dye, indicating that regardless of whether the AC is coated or embedded in the epoxy layer, it could be considered as a promising material for the removal of MB dye from aqueous solution. The surface integrity analyses, such as shaking method, were conducted and their results confirmed that granular activated carbon coating has been successfully deposited on the HDPE substrate and that there was no loss of carbon between Day 1 to Day 28.

Abstract ID: 731

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Theory of Structure, Surface and Interface of thin films

Keywords: Oxide Thin Films, Strain, Advanced Electron Microscopy

Structural investigation of (Pr_{0.5}Ba_{0.5}MnO₃)_{0.8}:(CeO₂)_{0.2} nanocomposite films prepared on (001) (La,Sr)(Al,Ta)O₃ substrates

Shao-Dong Cheng^{1,2}, Sheng Cheng², Lu Lu², Ming Liu², Shao-Bo Mi¹

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The perovskite-type manganites Ln_{1-x}Ba_xMnO₃ (Ln=lanthanide ion, such as La and Pr) have received significant attention because of their intriguing physics caused by the strong interplay between the lattice, charge and spin degrees of freedom. Among the manganites, half-doped Pr_{0.5}Ba_{0.5}MnO₃ exhibits excellent mixed ionic/electronic conductivity, fantastic magnetic properties, and transport features. In addition, cerium dioxide is an oxide conductor at high temperatures, and thus has been applied in solid oxide fuel cells. To achieve vertically aligned nanocomposites (VAN) thin films composed of perovskite-type manganites and cerium dioxide is of great importance since the functional properties of the VAN films can be tuned by lateral and vertical strain in the heterosystems.

In this work, (Pr_{0.5}Ba_{0.5}MnO₃)_{0.8}:(CeO₂)_{0.2} (PBMO:CeO₂) thin films were prepared on single-crystalline (001) (La,Sr)(Al,Ta)O₃ (LSAT) substrates by pulsed laser deposition (PLD). The structural properties have been studied by selected-area electron diffraction (SAED), high-angle annular dark-field (HAADF) imaging, and atomic-resolved energy dispersive X-ray spectroscopy (EDS) on JEOL ARM 200F microscope equipped with a probe aberration corrector and an Oxford X-MaxN 100TLE spectrometer, operated at 200 kV.

On the basis of low-magnification bright-field (BF) TEM observations, self-assembled VAN thin films formed on the LSAT substrates. Along the film growth direction, two types of crystallographic orientation relationship (OR) appear between PBMO and CeO₂, (001)[100]PBMO|| (001)[11 $\bar{0}$]CeO₂ and (001)[100]PBMO|| (100)[011 $\bar{1}$]CeO₂, which was determined by the SAED. HAADF observations on the VAN films show that the PBMO/CeO₂ lateral and vertical interface can be coherent and semi-coherent depending on the OR between PBMO matrix and CeO₂ nanopillars. For the semi-coherent PBMO/CeO₂ interface, the interfacial dislocations distribute regularly at the interface, which contributes to the strain relaxation in the VAN films. The lattice mismatch between the nanocomposite thin films and the substrate may lead to the formation of two types of OR in the VAN films. In addition, atomic-resolved EDS maps of the PBMO/CeO₂ lateral and vertical interfaces reveal that cation segregation occurs at the coherent PBMO/CeO₂ interface. Regarding the magnetization and magnetoresistance of the VAN thin films measured in this system, the structure-property in the PBMO:CeO₂ thin films were discussed in details.

Abstract ID: 732

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Invited Talk

Topics: Biodetection

Keywords: Frequency shift, Biomarker, MicroRNA, SERS, Liver cancer

Frequency Shift Raman-Based Sensing of Serum Biomarkers for Early Diagnosis and Discrimination of Primary Liver Cancers

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Frequency shift surface-enhanced Raman scattering (SERS) achieves multiplex microRNA sensing for early serological diagnosis of, and discrimination between, primary liver cancers in a patient cohort for whom only biopsy is effective clinically. Raman reporters micro-printed on plasmonic substrates shift their vibrational frequencies upon biomarker binding with a dynamic range allowing direct, multiplex assay of serum microRNAs and the current best protein biomarker, α -fetoprotein. Benchmarking against current gold-standard polymerase chain reaction and chemiluminescence methods validates the assay. The work further establishes the frequency shift approach, sensing shifts in an intense SERS band, as a viable alternative to conventional SERS sensing which involves the more difficult task of resolving a peak above noise at ultra-low analyte concentrations.

Abstract ID: 733

Symposium 5: Functional 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, Terahertz wave, Metamaterial

Manipulation of Terahertz Wave with Tunable Graphene Metamaterial Structures

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Graphene, a two-dimension material consisting of one monolayer of carbon atoms, has been recently applied in electronic and photonic devices due to its exotic properties, such as optical transparency, flexibility, high electron mobility. In addition, its sheet conductivity can be continuously tuned in a broad frequency range by shifting the electronic Fermi level via chemical or electronic doping, which enables fast electrical modulation and on-chip integration. This makes the continuous or structured graphene sheet a promising candidate for designing tunable terahertz (THz) metamaterial. Here, we show several design examples of combining the metamaterials having different unit cells of metallic resonator with the double layer graphene to realize THz devices that could manipulate the wave propagation. Firstly, a tunable THz energy absorber based on graphene metamaterial with polarization independence has been designed and analyzed. The absorption performance with a peak frequency tuning range of 15% and almost perfect peak absorption has been demonstrated by controlling the Fermi energy of the graphene that can be conveniently achieved by adjusting the bias voltage on the graphene double layers. Secondly, we present a THz dynamically tunable broadband metamaterial polarization rotator composed of two metal gratings and two orthogonal graphene grating structures as well as the dielectric spacers. By applying different bias voltages to adjust the Fermi energy of graphene, this rotator can conveniently rotate the polarization direction of the linearly polarized incident light by any desired angle among a wide range from 20 to 70 degree in transmission mode. Finally, we propose a tunable metasurface consisting of metallic patch array on a grounded polymer substrate embedded with graphene layers to electrically control the electromagnetic beam reflection at THz frequency. We demonstrate that either single beam or dual beam dynamically switching between normal and oblique reflection angles can be well attained at working frequency. These proposed approaches may bring much freedom in the design of THz devices and may be applied to dynamic control of THz wave propagations.

Abstract ID: 734

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Ceramic based composites

Keywords: 0.95MgTiO₃-0.05CaTiO₃, ZnO-Yb₂O₃ co-doping, dielectric performances

Influence of ZnO/Yb₂O₃ doping of (Mg_{0.95}Ca_{0.05})TiO₃ ceramics on their sintering characteristics and microwave dielectric properties

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The phase composition, as well as microstructure and microwave dielectric characteristics of 0.95MgTiO₃-0.05CaTiO₃ (95MCT), composite doped with different amounts of Yb₂O₃/ZnO that had a great improvement on 95MCT, was researched. The optimum amount of Yb₂O₃ and ZnO could effectually impede the formation of the second phase in 95MCT. The Yb₂O₃/ZnO co-doping helped to eliminate the pores inside 95MCT and made the microstructure denser. Doping Yb₂O₃/ZnO into 95MCT ceramics could expand the sintering temperature range and lower the sintering temperature, at which 95MCT ceramics with the higher density could be acquired. What's more, the $Q \times f$ value had been improved greatly by using Yb₂O₃/ZnO co-doped. The microwave characteristic of 95MCT doped with x wt% Yb₂O₃ + $(2 - x)$ wt% ZnO ($x = 0.2, 0.5, 1.0, 1.5$) was studied. When $x = 1$, the microwave properties of 95MCT ceramics were the best: the best dielectric constant ϵ_r of 20.89, a optimum τ_f of $-2.03 \text{ ppm} \cdot ^\circ\text{C}^{-1}$ and a maximum $Q \times f$ value of 67800 GHz (7GHz).

Abstract ID: 735

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Design and application of composite structures

Keywords: First-Principles Simulation, Photocatalyst/Catalyst, Electric Dipole

Energy Material Design Based on Electric Dipole Simulations

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Using first-principles calculations at the density functional theory (DFT) level, we have proposed that the electric dipole, a parameter deduced from the distribution of ground or excited states, is a useful descriptor to describe and evaluate the structure-property relationship of energy materials. It helps to understand the electron kinetics in for various physics or chemistry applications, and thereby enable the manipulation of electron-photon interactions, energy/electron transfer, and material conversion processes. By developing quantum chemistry and deep learning techniques to compute the electric dipole moment, we have demonstrated it as an efficient knob to improve the rational design of photocatalyst, catalyst, solar cell, smart materials, and so on.

Abstract ID: 736

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Advances in the Synthesis and Characterization of low dimensional, nano and 2D materials

Keywords: Graphene electrode, Copper nanocrystals, Catalysts, Biosensing

Control of the Size and Chemical Composition Selective Copper Nanocrystals on Highly Conductive Graphene Sheet Electrode

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Flexible conductive graphene is an excellent electrode material for versatile applications. In this study, a systematic investigation of deposition of copper nanocrystals onto graphene sheet electrodes using a simple electrochemical method has been carried out. By changing the potential of the electrodeposition, an optimized narrow window of sub-100 nm sized nanocrystals can be effectively produced exclusively. By analysing their current-time transient profiles, a clear transition from predominantly instantaneous to predominantly progressive nucleation growth mechanism is found, consistent with scanning electron microscopy observation of their morphological evolution. In addition, a combination of the X-ray diffraction and X-ray photoelectron spectroscopy results show that different deposition potentials alter not only the deposited nanocrystal sizes and shapes but also the chemical compositions of nanocrystals. Metallic copper crystals and cuprous copper oxide crystals can be produced by carefully selecting different deposition potentials and temperature. This finding paves a direct pathway to selectively manufacture either metal or metal oxide nanocrystals designed for targeted applications in biosensing, photovoltaic and photocatalytic applications.

Abstract ID: 737

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Multifunctional composites

Keywords: Phosphor, Sensor, Visualization

Stable Chromaticity of Red Titanate Phosphors for Sensor and Visualization

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Phosphors are traditionally used for lighting applications, actually, they also have a high potential for sensor and visualization applications, for example, contactless temperature sensing and latent fingerprint identification. The method used to synthesize the phosphors is important, which critically influences the luminescence performance of the phosphors. Meanwhile, since the doping of a specific activator is required in order to produce the desired emission, activators with a high chemical stability and ecofriendly preparation procedure are preferred, such as Mn⁴⁺ transition metal ions. In this study, titanate phosphors doped with red activators were prepared using solid-state reaction and sol-gel method. Possible phase transitions during heating were analyzed. The prepared phosphors showing single-phase or bi-phase were dependent on the synthesis approaches, and were resulted in different luminescence efficiencies. Crystallinity and crystalline structure of the synthesized titanate phosphors were investigated and discussed with the high-resolution images. We found that the phosphors showed similar photoluminescence patterns and stable chromaticity even though the working conditions were varied. Furthermore, the red titanate phosphors achieved stable thermometry over a wide temperature range, and performed with a high absolute sensitivity and relative sensitivity at 393 K. The titanate phosphors also showed good performance as a fluorescence label for latent fingerprints visualization on various substrates. Clearly, this multifunctional titanate phosphors show a high potential for life application.

Abstract ID: 738

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Plenary**

Topics: Piezotronics for smart systems

Keywords: Multiaxial, Molecular Ferroelectric, Quasi-spherical Theory, Symmetric Broken

Multiaxial Molecular Ferroelectric material

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Molecular ferroelectrics are attracting much attention because of their low cost, light weight, easy processing, mechanical flexibility, environmentally friendliness and outstanding performance. Although the history of ferroelectrics began with the first molecular ferroelectric Rochelle salt in 1920, most of the molecular ferroelectrics are uniaxial and particularly difficult to find appropriate substrates for growing high-quality epitaxial or single-crystalline films of uniaxial molecular ferroelectrics. It is of fundamental importance to introduce multiaxial nature into molecular ferroelectric to make the polarization switched between multiple directions, facilitating the application in polycrystalline thin-film form, similar to the inorganic ferroelectric ceramics. During years of searching for new molecular ferroelectrics, we developed an effective “quasi-spherical theory” design strategy to construct multiaxial molecular ferroelectrics. The quasi spherical molecule based crystal structure in the ferroelectric phase is easy to have low crystal symmetry to satisfy the molecular symmetry, and then become a spherical one with high molecular symmetry in the para-electric phase to result in a very high symmetry crystal structure. The significant crystal symmetry change in the paraelectric-to-ferroelectric phase transition will then induce the multiaxial feature. Based on this strategy, we selected quasi spherical cation to construct a series of multiaxial molecular ferroelectric, all of which became spherical ones in the paraelectric phase. We believe this fine molecular design strategy will enrich the family of multiaxial molecular ferroelectric, and promote the practicable applications of molecular ferroelectrics.

Abstract ID: 739

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Photonic and optoelectronic device applications of low dimensional, nano and 2D materials

Keywords: Two-dimensional materials, Van der Waals heterostructures, Optical modulators, Nonlinear optics, Ultrafast laser

Two-dimensional layered materials based van der Waals heterostructures and their applications for broadband optical modulators

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Recent advances in the growing two-dimensional layered materials (2DLMs) and stacking different 2DLMs to form van der Waals heterostructures (vdWhs) have provided approaches for the preparation of functional devices in the ultimate two-dimensional limits. The previous researches have demonstrated that vdWhs could modulate the electronic band structure of the materials and lead to the adjustment of their nonlinear optical properties. However, the influence for nonlinear optical properties of the vdWhs such as various stacked orders, thickness and different materials has not been investigated experimentally. Herein, we systematically investigate the effect of nonlinear optical properties of vdWhs by engineering their structures. We grow different 2DLMs with large area, uniform thickness and high crystal quality by chemical vapor deposition method and then vertically stack them in turns on sapphire substrates. Then we systematically investigate their nonlinear optical properties by utilizing z-scan technique under different probe wavelengths (800 nm, 1560 nm) and carrier relaxation property using pump-probe technique. After preparing vdWhs based optical modulators, we further study their nonlinear saturable absorption properties by utilizing balanced two-twin detectors equipment at 2 μm wavelength and then embedding them into two types fiber laser systems (Erbium-doped and Thulium-doped fiber laser systems) to investigate their ability in stable pulse generation. The results demonstrate that vdWhs based optical modulators own broadband operation ability ranging from 800 nm to 2 μm and the nonlinear saturable absorption properties (such as saturable intensity and modulation depth) could be engineered in a large range. These features suggest the feasibility of engineering broadband optical modulators using vdWhs for desired photonic devices.

Abstract ID: 740

Symposium 3: Functional Catalysis (FC)

Invited Talk

Topics: Photocatalysis

Keywords: Wastewater treatment, Photocatalysts, Biotemplated, Mesoporous materials, Photocatalytic reactor

Biotemplated Mesoporous Materials Based Photocatalysis for Water and Wastewater Treatment

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One of the problems that people in developing countries are facing is the abundance of organic micro-pollutants and heavy metals in natural water resources. Therefore, low-cost drinking water treatment technologies removing contaminants to reduce waterborne diseases, and to prevent dangerous chronic diseases (including cancer) are needed before pumping to the families in remote mountainous areas. On the other hand, the scale-up of photocatalytic reactors for the wastewater treatment with high COD (200mgL⁻¹) is still a big challenge though photocatalytic processes involving TiO₂ semiconductor particles under UV light illuminations have been shown to be potentially advantageous and useful in the treatment of wastewater such as dye effluents.

Mesoporous materials with tunable pore structure and tailored property have great potential as photocatalysts and adsorbents for wastewater treatment. In this presentation, biotemplate such as plant tissues, algae, natural rubber latex and botanic extracted pigments were employed for preparation of mesoporous materials. These materials could be used for effective photocatalytic degradation of organic pollutants and photocatalytic reduction of Cr⁶⁺, oxidation of As³⁺. They were also used as adsorbents for removal of PO₄³⁻ in wastewater. Proposed advantages and prospects of the pilot-scale photocatalytic reactors based on biotemplated mesoporous photocatalysts are also discussed.

I will focus on photocatalytic disinfection, treatment of raw water, high turbidity water or with high concentration of algae, mercury, arsenic, phosphate, and nitrite removal technologies. Hopefully, we will provide combined equipments and technical support for more drinking water purification in remote areas in the world.

Furthermore, the lessons and experience we obtained in the development of photocatalytic reactors for wastewater treatment including lignite gasification wastewater, tobacco wastewater, wastewater at expressway service area and hospitals will be given.

Abstract ID: 741

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Natural biomaterials

Keywords: Biopolymer, Cryoprotective agent, Antarctic microorganism

A novel Anti-freezing Biopolymer derived from Antarctic Microorganism as Cryoprotective Agent

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Cryopreservation is closely related to clinical and biotechnology field and is widely used to extend the viability of cells or tissues. The various physical and chemical processes that occur during the freezing and thawing process are the factors that make it difficult to cryopreserve biological materials such as mammalian cells and tissues. The major cause is crystallization by water, and water crystal damages the cell membrane, so that most cells die during the freezing process. Several types of cryoprotective agents (CPAs) have been developed to increase the biological survival rate of cryopreservation from these factors. Currently widely used CPAs, such as glycerol or dimethyl sulfoxide (DMSO), can cause toxic or other chemical effects on the cell, so should be removed from the cell prior to research or clinical use. Bacteria that survive in polar environments secrete Exopolysaccharide (EPS) to survive in cold environments, some of these polymers are known to have anti-freezing properties. We have found an anti-freezing biopolymer, an inhibitor of ice growth, from the marine microorganism, *Pseudoalteromonas* sp Strain CY01 in the Antarctic Ross Sea. The following study was conducted to demonstrate the effect of this biopolymer on blood cryoprotection.

As a result of adding 2.5% A-CPA to confirm the protective effect of erythrocytes (RBC), the hemolysis ratio of RBC decreased significantly from $92.48 \pm 6.69\%$ to $9.08 \pm 0.37\%$. In order to confirm the long-term preservation ability of A-CPA, hemolysis ratio was $7.24 \pm 2.15\%$ after storage for 5 months at $-80\text{ }^{\circ}\text{C}$. In addition, ATPase levels were measured after freezing and thawing using A-CPA to determine cell activity after freezing. As a result, there is no changed ATP level before freezing ($2.50 \pm 0.06\text{ }\mu\text{M}$) and after thawing ($2.26 \pm 0.19\text{ }\mu\text{M}$). Next, to compare the 2,3 DPG values (the oxygen saturation index) of RBC, 2,3 DPG values showed statistically no changes from $4.26 \pm 0.24\text{ }\mu\text{M} / \text{g Hb}$ before freezing to $3.98 \pm 0.47\text{ }\mu\text{M} / \text{g Hb}$ after thawing. However, when treated with PBS, the levels of ATP and 2,3 DPG were significantly reduced to $0.18 \pm 0.02\text{ }\mu\text{M}$ and $0.78 \pm 0.92\text{ }\mu\text{M} / \text{g Hb}$, respectively. The supercooling point of A-CPA was $-32.1 \pm 0.02\text{ }^{\circ}\text{C}$, which was much lower than that of 1% glycerol and 1% DMSO mixture at $-14.2 \pm 1.2\text{ }^{\circ}\text{C}$.

A-CPA 1) can be replaced or reduced the use of existing toxic DMSO, and 2) has potential as a new cryoprotectant that can eliminate the essential cleaning process when using glycerol for blood preservation. Moreover, biopolymers extracted from microorganisms are regarded as safe and can be used in various fields in medicine, pharmacy, veterinary science and biotechnology in near future.

Abstract ID: 742

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Nanomaterials for Photonics and Optoelectronics

Keywords: Chemical combustion method, PL excitation, CIE chromaticity diagram and display devices

Violet-blue-shift of spectrum and enhanced luminescent properties of $\text{Ca}_3(\text{PO}_4)_2:\text{Ce}^{3+}$ phosphor induced by small amount of Gd^{3+} incorporation

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$\text{Ca}_3(\text{PO}_4)_2:1\text{Ce}^{3+}/x\text{Gd}^{3+}$ (where $x=0.5, 1.0, 3.0$ and 7.0 mol%) phosphors were synthesized by a convention chemical combustion method. The X-ray diffraction (XRD) patterns showed their rhombohedral structure with space group of $R\bar{3}c$, and several diffraction peaks shifted to lower angle side when co-doped with Gd^{3+} ions. Field emission scanning electron microscopy images exhibited irregular spherical particles in micrometer range. The optical properties including reflectance, excitation and emission were investigated. The band gap of the phosphors was calculated from diffuse reflectance spectra data using the Kubelka–Munk function. The PL excitation (PLE) spectra exhibited the broadband $4f-5d$ transition of Ce^{3+} ions centered at 439 nm. The photoluminescence (PL) properties of the $\text{Ca}_3(\text{PO}_4)_2:\text{Ce}^{3+}/\text{Gd}^{3+}$ phosphors were studied as a function of the Gd^{3+} ion concentration. The $\text{Ca}_3(\text{PO}_4)_2:\text{Ce}^{3+}/\text{Gd}^{3+}$ phosphor had a wide emission band ranging from blue to yellow peaking at 532 nm, due to the transition from the lowest $5d$ band to $2F_{7/2}, 2F_{5/2}$ states of the Ce^{3+} ion. The PL spectra showed the intense $5d-4f$ transition of the Ce^{3+} ions with a band maximum at 542 nm, and this band maximum shifted to the longer wavelength region by increasing concentration of the Gd^{3+} ion. The CIE chromaticity diagram showing emission colour tuning in $\text{Ca}_3(\text{PO}_4)_2:\text{Ce}^{3+}/\text{Gd}^{3+}$ phosphors from violet to violet-blue when co-doped with Gd^{3+} ions. The present phosphor can acts as a novel host material for violet-blue emission for display devices, phototherapy and photoluminescent liquid crystal displays.

Abstract ID: 743

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Bioengineering film

Keywords: Coating, Citrus, Functional textiles, waste recycling

Coating of Citrus Cellulosic Extracted from Citrus Waste on Fabric for Technical Applications

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The aim of this study is to extract cellulose from peel waste of commonly grown citrus fruit named Citrus Reticulata, which is also commonly known as Kinnow. It is widely cultivated in Punjab region of Pakistan and India. It is a high yield mandarin, hybrid of two citrus cultivars, Willow Leaf and King. Kinnow is classified as King of all varieties of easy peelers and considered as the best variety in the world. The juice content in mandarin is about 44% to 47.5%, which is highest in all easy peeler varieties. Citrus fruits are consumed directly as fruits as well as for fresh and concentrated juices. The residue left after juice extraction contain valuable materials which needs to be regenerated to produce goods. As a rough estimate, more than half weight (52.5%) of the citrus fruit is wasted after juice extraction which is used for animal feeding or for burning in furnaces. This largely available raw material can provide value added products through processing and will easily attract investors to develop new industries. Citrus peel contains about 12.7% to 13.6% cellulosic content in it. The extraction of cellulose will provide cheap raw material for different industries including food, paper and pulp and textiles.

In this study, cellulose has been extracted from citrus peel waste. The process starts with steeping process followed by churning process and extraction by filtration process at the end. The obtained extracted cellulose was further coated on fabric through dip, dry and cure technique. The analytical testing of the samples includes Scanning Electron Microscope and Fourier Transform Infrared Spectroscopy. The washing fastness of the coated fabric samples were carried out at three different washing intervals from 40-60 cycles. The obtained FTIR results confirmed that cellulose was successfully extracted from citrus peel waste. The SEM image of coated fabric is shown in Figure 1(a). It is clear from the results that cellulose was successfully coated on the fabric using dip, dry and cure method. The washing fastness of the coated cellulosic content was also analyzed using standard detergent at 40 cycles, 50 cycles and 60 cycles. The results confirmed that cellulose was firmly attached with viscose fabric as shown in Figure 1(b-d). The FTIR results confirms the presence of ascorbic acid as additional functional material for technical applications of coating.

The obtained results concluded that citrus peel waste can be successfully used to regenerate cellulose from it for further processing and usage. The extracted cellulose can be used to develop fiber, coating, films or any other useful application. The inclusion of vitamin C in coating will be functionally used for vitamin deficit patients in medical textiles. In such regards, environmental friendly process can be designed to reuse the waste products and support to build a better world.

Abstract ID: 744

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin Film Growth & Epitaxy

Keywords: Double-Perovskite Films, Growth Temperature, Interface Strain, B-site ordering

Temperature-dependent B-site ordering in double-perovskite La₂NiMnO₆ films

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The multiferroic double-perovskite La₂NiMnO₆ (LNMO) has been considered as a promising candidate of ferromagnetic semiconductor for magnetoelectronics and spintronics due to its high paramagnetic-to-ferromagnetic curie temperature (~280 K) and good magnetic properties near room temperature [1-3]. In addition, the crystallographic ordering and oxidation states of the B-site cations (Ni and Mn) in LNMO related to the nature of the ferromagnetism have been attracted much research attention. Nowadays, based on aberration-corrected electron microscopy, advanced imaging techniques in combination with atomic-resolution energy-dispersive X-ray spectroscopy (EDS) mapping provide us with unrivaled capability to understand the structural and chemical properties of materials at the atomic scale.

In this work, the effect of growth temperature on the B-site cations ordering in LNMO thin films grown on different substrates, SrTiO₃, (La,Sr)(Al,Ta)O₃, KTaO₃ and LaAlO₃ has been systematically investigated by using advanced electron microscopy techniques [4,5]. It is found that the ordering of B-site cations in LNMO films could be affected by controlling film-growth temperature. For instance, the LNMO films grown at 800 °C are partially disordered, while the LNMO films prepared at 900 °C exhibit a long-range B-site ordering. In addition, our work indicates that LNMO films under tensile strain exhibit a monoclinic structure, while under compressive strain the crystal structure of LNMO films is rhombohedral. It should be noted that the ordering of B-site cations is independent of the epitaxial strain. The atomic-scale characterization of chemical and structural properties of multiferroic LNMO films would extend our understanding of the process-structure-property relationship in the materials and explore their potential applications.

Abstract ID: 745

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Solar Cells

Keywords: Renewable energy, Photovoltaic, Solar cell, sub-Saharan Africa, Energy materials

The Significance of Domestic Production of Low-Cost Photovoltaic Cells in Sub-Saharan Africa Renewable Energy Roadmap and Wellbeing

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Studies have shown that sub-Saharan Africa (SSA) has the highest number of people without access to electricity and also doubled as the region with the least rate of power access. Consequently, the region has the highest share to world's poverty, which has multi facet implications on the region's economy and the wellbeing of the people. The region dominates global unemployment, the use of biomass for cooking, and health issues related to the use of unclean energy charts. Despite this ugly situation, the region is not forthcoming in the active participation and implementation of the contemporary renewable and transition energy programmes. Hence, the study x-rays the status of renewable energy deployment and the benefits of building an active domestic capacity in the development of low-cost photovoltaic cells in SSA. Active participation in the domestic research and manufacturing of energy materials, such as batteries, supercapacitors, fuel cell and photovoltaic panel in SSA will make low-cost PV systems available in the region and this will facilitate – increase access to affordable and clean power; creation of jobs; reduce the consumption of fossil fuels; greenhouse (GHG) emissions reduction; diseases caused by biomass usage reduction; fight against poverty; and powering of pump for agriculture and desalination units.

Abstract ID: 746

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Keynote

Topics: Biomaterials for soft tissue applications

Keywords: Graphene, Scaffold, Neural Stem Cell, AD therapy

3D graphene scaffolds meets neural stem cells

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Neural stem cells (NSCs) based therapy provides a promising approach for neural regeneration. For the success of NSC clinical application, a scaffold is required to provide three-dimensional cell growth microenvironments and appropriate synergistic cell guidance cues. Here, we report the first utilization of graphene foam, a three-dimensional porous structure, as a novel scaffold for NSCs in vitro. It was found that three-dimensional graphene foams (3D-GFs) can not only support NSC growth, but also keep cell at an active proliferation state. Meanwhile, phenotypic analysis indicated that 3D-GFs can enhance the NSC differentiation towards astrocytes and especially neurons. Furthermore, a good electrical coupling of 3D-GFs with differentiated NSCs for efficient electrical stimulation was observed.

In this talk, I will address the effects of 3D dimensionality, stiffness and topological parameters for the underlying graphene scaffold on the proliferation and differentiation of adult neural stem cells. Alzheimer's disease model both in vitro and in vivo was established to elucidate the possibilities and challenges of neural stem cell therapy. Our findings implicate 3D-GFs scaffold offer a powerful platform for NSC research, neural tissue engineering and regenerative medicine.

Keywords: Graphene, Scaffold, Neural Stem Cell, AD therapy

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Abstract ID: 747

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

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

Keywords: Diketopyrrolopyrroles, organic semiconductors

**Exploring Structure Based Charge Transport Relationships in Phenyl
Diketopyrrolopyrrole Single Crystals Using a 2D π - π Dimer Model System**

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Achieving optimal charge carrier mobility in small molecule π -conjugated organic semiconducting architectures, where one and two-dimensional π -stacking motifs represent desirable charge propagation channels is at the forefront of current research interests and efforts.^{1–3} In this regard, crystalline phenyl diketopyrrolopyrroles are often overlooked as charge transfer mediating materials in optoelectronic applications.⁴ However, we have recently demonstrated that in turn, phenyl DPP based architectures represent theoretically superior alternatives to their furan and thiophene-based counterparts.^{5,6} Herein, we report an experimentally ratified two dimensional π - π model dimer systems dispelling previous misconceptions regarding their potential as organic semiconductors and that will enable researchers to screen and predict charge transport potential solely on the basis of their single crystal derived π -stacking architectures. In testing our model system versus the available database of phenyl diketopyrrolopyrrole single crystal structures we reveal that these materials are characterised by intrinsically large thermal integrities and in many cases large charge transfer integrals, not solely restricted to dimeric interactions exhibiting close intermonomer arrangements and bearing low torsion of the core phenyl rings. It is envisaged that this study will be of significant interest to the increasingly large community engaged in the quest to engineer π -conjugated organic based semiconducting devices and particularly those employing crystalline diketopyrrolopyrroles.

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Thursday, 22/Aug/2019 8:36am - 8:48am

Abstract ID: 748 / FESC: 4

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: supercapacitors, small-angle X-ray scattering, in-situ studies

Watching ions in nanoporous supercapacitor electrodes at work using in-situ small-angle X-ray scattering

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Supercapacitors are energy storage devices for applications requiring high power density and long cycle lifetime. They store charge purely physically in an electrical double-layer at the electrode-electrolyte interface within highly porous carbon electrodes. In this lecture we will demonstrate that in-situ small-angle X-ray scattering (SAXS) in combination with in-situ X-ray transmission (XRT) and electrochemical measurements are promising methods to study global ion fluxes and local ion arrangements within meso-/microporous carbon electrodes during charging [1]. However, the interpretation of SAXS data from such complex multicomponent systems is challenging. We developed new methods of SAXS data analysis using an atomistic modelling approach, allowing far-reaching interpretation of ion storage mechanisms and related predictions about optimized carbon nanostructures [2]. The approaches are also suitable to study ion dynamics, notably the discrimination between different mechanisms such as ion exchange, counter-ion adsorption or co-ion expulsion [3]. In this respect, XRT is a very simple, yet extremely powerful method, which can be easily done at laboratory X-ray sources. However, there are several assumptions and approximations involved, which can be verified using synchrotron radiation based anomalous small-angle X-ray scattering (ASAXS) to obtain local ion-specific information during charging.

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Thursday, 22/Aug/2019 4:27pm - 4:39pm

Abstract ID: 749 / FESC-2: 13

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: Graphene oxide, Polypyrrole, Textiles, Reactive inkjet printing, Supercapacitor

Flexible solid-state supercapacitors based on graphene/polypyrrole composites inkjet printed on textile substrates

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Rapid development of smart textiles and wearable electronics requires a new generation of energy storage devices. Among the many energy storage devices available, flexible supercapacitors are promising candidates because of their quick charge-discharge capabilities and long life cycles. In this work, we report a novel method to fabricate a solid-state supercapacitors based on reactive inkjet (RIJ) printing of graphene/polypyrrole composites on polypropylene (PP) nonwoven fabric. The flexible solid-state supercapacitors were fabricated through a three-step approach. First, two gold current collectors were deposited onto the PP nonwoven fabric by using physical vacuum deposition. Next, two rGO/PPy electrodes were deposited on gold current collectors by using the RIJ printing. During printing, three print-heads were used, where the first print-head was filled by aqueous solution of pyrrole (Py) in the concentration of 0.6 M, the second one by aqueous solution of ammonium peroxydisulfate (APS) in the concentration of 0.6 M and third one by graphene oxide dispersion in water (5 g/L). The rGO/PPy electrodes were deposited line by line onto the PP fabrics in such a way that the first nozzle sprayed the selected line of pattern using an aqueous solution of Py, next the second nozzle sprayed the same line using an aqueous solution of APS and then the third nozzle sprayed the same line using a GO dispersion. The presented method allowed for in-situ synthesis of PPy and removing most of the oxygen functional groups from the surface of graphene, providing a layer with high conductivity. Finally, two PP/Au/rGO/PPy hybrid structures were immersed into PVA/H₃PO₄ aqueous solution and solidified together thereafter, with a separator sandwiched between them. The electrochemical performances of the assembled supercapacitors were investigated by cyclic voltammetry (CV), constant current charge/discharge (CCCD) tests, and electrochemical impedance spectroscopy. The CV curves showed that supercapacitors exhibited a quasi-rectangular profile with quite current responses at the beginning of positive and negative potential scans and a good capacitive feature with rapid diffusion and adsorption of electrolyte ions onto porous rGO/PPy electrodes. CCCD curves at various currents in a voltage window of 0 - 0.8V exhibited that the charge curves are almost symmetric to its corresponding discharge counterparts. A low voltage drop of ca. 50 mV was noted for the charge/discharge current equal to 1 mA. On the base of the CV curves, the areal and gravimetric capacitance vs scan rate was calculated. It was, respectively, from 0,15 to 0,74 F/cm² and 113 to 553 F/g in dependence of scan rate.

Abstract ID: 750

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Green Composites

Keywords: Conducting polymers, Nanofunctional polymers, Green Chemistry, Nano composites

Microwave synthesized conducting polymer-based green nano composites as smart materials

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The Green Chemistry and Engineering focusses to improve the present globe today and for future generations by imparting sufficient pioneering solutions and practices to accomplish sustainability challenges, while simultaneously fulfilling social, economic, and environmental goals. This green arena includes Polymer Science of functional materials in which conducting polymers (CPs) are considered a promising prospect due to their exhilarating creative properties. Thus, they have developed as one of the most eminent members in this field. The new promising technology of using Microwave (MW) radiations for synthesis and processing using MW-assisted heating, under controlled conditions is a valuable technology for CPs as well. The significant reduction in their reaction times-typically from days or hours to minutes or even seconds. The work reports the role of conducting polymers and nanocomposites, with their broad applications as nanocomposites synthesized by green approach viz. microwave irradiation and their significant contribution in materials science and engineering as a whole and green chemistry particular, with their emerging prospects. Herein, we have synthesized conducting Poly(p-phenyldiamine) (PPDA) via MW, following seven principles of “green chemistry” approach. This includes less hazardous chemical synthesis, atom economy, prevention, safer solvents, design as energy efficient process, reduction of side products and remarkably, eco-friendly nature. The use of aqueous medium during synthesis process proved to be green, renewable and free from harmful VOCs. We have also analyzed the effect of MW irradiation on various properties of Poly(p-phenyl-diamine) (mPPDA) and its comparison with conventionally polymerized PDA (cPPDA). The FT-IR, TEM, SEM-EDX, and four-probe conductivity measurements were performed to analyze and account the influence of MW irradiation on the morphology, size, solubility, and electrical properties. This study insights the viable and facile synthesis for developing high-performance conducting nanomaterials for electromagnetic shielding applications (EMI shielding).

Abstract ID: 751

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Applications of Biopolymer for Drug Delivery

Keywords: Prodrug, triggered release, chemotherapy

Zein-paclitaxel prodrug nanoparticles for redox-triggered drug delivery and enhanced therapeutic efficiency

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Prodrug is one of the main strategies to target the disease site to improve the drug efficiency and reduce the adverse effects of chemotherapy. Because of the good capability of chemical modification, zein, a plant derived protein, and drugs can be conjugated through environmentally sensitive links to form prodrugs capable of triggered drug release. In this study, a novel prodrug was synthesized using paclitaxel (PTX), zein, and a disulfide linker, and nanoparticles were formed by self-assembly of the prodrug. In vitro triggered drug release was studied and the drug cytotoxicity were examined using both cancer and normal cells. In vivo antitumor activity was studied using tumor xenograft animal model. An effective in vitro triggered release, 80– 90% in 5 min, of the prodrug based nanoparticles (zein-S-S-PTX_NP) was successfully approached. The cytotoxicity of zein-S-S-PTX_NP as well as the zein encapsulation of PTX (zein_PTX_NP) and pure PTX on HeLa cells and NIH/3T3 fibroblast cells was tested using MTS assay. It showed that, after the treatment of zein-S-S-PTX_NP at the equivalent PTX concentrations of 0.1, 0.5, 1, and 5 μ g/mL, respectively, zein-S-S-PTX_NP had zero damage to normal cells but a similar cytotoxicity to cancer cells as pure PTX. In the animal study, the tumor was 50% of the original size after the treatment of zein-S-S-PTX_NP for 9 days with 3 doses. This study suggested that the novel prodrug based nanoparticle zein-S-S-PTX_NP could be a promising approach in chemotherapy with targeted delivery, improved efficacy, and reduced side effects.

Abstract ID: 752

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Theoretical/Modelling/Computer Simulations Of Functional Materials

Keywords: Thermoelectrics, Figure of merit, Energy filtering, Stabilization, Boltzmann Transport theory.

Theoretical investigations on Stabilization of thermoelectric figure of merit for Bulk nanostructured PbTe System.

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This work presents theoretical investigations on the stabilization of thermoelectric figure of merit (ZT) over a broad range of temperature for Bulk nanostructured p-type PbTe material. The Bulk nanostructured materials are either nanoparticles embedded in matrix or periodic (or aperiodic) array of nanostructures. These nanoinclusions or granular structures provide interfaces of certain barrier height and width. The ZT which is directly proportion to (Power factor X Temperature) and inversely proportional to the thermal conductivity gets stabilized due to filtering of low energy carriers by these interfaces. We perform theoretical calculations using Boltzmann Transport theory to find optimized barrier height and width for which ZT is stabilized over a wide range of temperature. Experimentally these optimized barrier height and width can be achieved by choosing the appropriate material and size of nanoinclusions or by varying the distance between granular structures. Our theoretical calculations show that, at optimized barrier height and width, Power factor decreases with temperature but the product of Power factor and temperature remains nearly constant. Also, the thermal conductivity varies slowly with temperature thus resulting in stabilized ZT for a wider range of temperature.

Abstract ID: 753

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Electrochemical Supercapacitors

Keywords: Polyaniline, Activated carbon fiber, capacitance, Wire-shaped microsupercapacitor, Pore structures

Electrochemical capacitance performance of polyaniline/activated carbon fibers

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A binary composite material of polyaniline/activated carbon fibers (PANI/ACFs) was developed as binder-free electrode material for energy storage. ACFs with optimized pore structures and oxygen-containing functional groups were prepared by physical activation and thermochemical treatment. PANI/ACFs was then obtained by depositing PANI nanowires onto ACFs substrate through an electro-polymerization process, showing nanowire-interconnected network structure. Well-designed PANI/ACFs benefited a directional electron transfer along with ACFs substrate during an electrochemical reaction process. The interface layer between ACFs substrate and PANI could act as the buffer space to restrain the volumetric change of PANI during the cycling charge-discharge process. The specific capacitance was improved from 325.8 F g⁻¹ for bare PANI/CFs up to 713.7 F g⁻¹ for PANI/ACFs at 1.0 A g⁻¹ in 1.0 M H₂SO₄ electrolyte. The rate capability was enhanced from 72.4 % for PANI/CFs to 83.2 % for PANI/ACFs as the current densities increased from 1.0 A g⁻¹ to 10 A g⁻¹. The capacitance retention ratio was enhanced from 60.4% for PANI/CFs film to 91.2% for PANI/ACFs after 4000 cycles even at a high current density of 5 A g⁻¹. All-solid state wire-shaped microsupercapacitor was also constructed using PANI/ACFs as a positive electrode, TiN wire as a negative electrode and sulfuric acid-polyvinyl alcohol gel as the electrolyte with the high output voltage of 1.6 V. So, PANI/ACFs can act as the promising electrode material for effective energy storage application.

Abstract ID: 754

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Biomaterial surfaces

Keywords: biosensor, Debye length, field-effect transistor (FET), label-free, serum, thyroid-stimulating hormone (TSH)

Direct, label-free and rapid transistor-based immunodetection in whole serum

Oscar Gutierrez-Sanz, Nesha M. Andoy, Marcin S. Filipiak, Natalie Haustein, Alexey Tarasov

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Transistor-based biosensors fulfill many requirements posed upon transducers for future point-of-care diagnostics devices such as scalable fabrication, label-free and real-time quantification of chemical and biological species with high sensitivity. However, the short Debye screening length in physiological samples (<1 nm) has been a major drawback so far, preventing direct measurements in serum. In this work, we demonstrate how tailoring the sensing surface with short specific biological receptors and a polymer polyethylene glycol (PEG) can strongly enhance the Debye length. The mechanism is explained in terms of local desalting of the sample by the polymer layer. In addition, the sensor performance can be dramatically improved if the measurements are performed at elevated temperatures (37°C instead of 21°C). With this novel approach, highly sensitive and selective detection of a representative immunosensing parameter -- human thyroid-stimulating hormone -- is shown over a wide measuring range with sub-picomolar detection limits in whole serum. To our knowledge, this is the first demonstration of direct immunodetection in whole serum using transistor-based biosensors, without the need for sample pre-treatment, labelling or washing steps. The presented sensor is low-cost, can be easily integrated into portable diagnostics devices, and offers a competitive performance compared to state-of-the-art central laboratory analyzers.

Abstract ID: 755

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Invited Talk

Topics: Advances in Enzymatic and Non-Enzymatic Biosensors

Keywords: α -endosulfan, pesticide, electrochemical sensor, CuO nanoparticles, nanointerface

Stalling Behaviour of Chloride ions: A Non-enzymatic Electrochemical Detection of α -Endosulfan using CuO Nano-interface

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Excessive and unsafe usage of pesticides lead to adverse effect on human beings, plants, animals and aquatic life. Endosulfan, categorized as class-I pesticide by World Health Organization, is a highly toxic pesticide, which is currently being used across countries though it has been banned. In this context, a non-enzymatic electrochemical sensor with copper oxide interface has been developed to detect α -endosulfan in water samples. Hydrothermal synthesized CuO nanospheres were characterized using X-ray Diffractometer, Scanning Electron Microscope and X-ray Photoelectron Spectrometer. CuO nano-interface modified gold working electrode along with Pt counter electrode and Ag/AgCl reference electrode were employed to carry out Differential Pulse Voltammetry (DPV) and amperometry studies to detect the presence of α -endosulfan in water. The stalling behavior of chloride ions present in α -endosulfan in reducing the current intensity confirmed the presence and concentration of α -endosulfan. The impedance variation for the varying concentration of α -endosulfan confirmed the proposed sensing mechanism. The sensor showed a linear range of 4-20 nM, and sensitivity of 0.03 μ A nM⁻¹. The relative standard deviation for the repeatability and reproducibility was 1.69%. The stability of the developed biosensor was 80.93% for 15 days.

Thursday, 22/Aug/2019 10:06am - 10:18am

Abstract ID: 756 / FCM-2: 11

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: PbTe nanocubes, micro-sheet, nanocomposite, thermoelectric, energy barrier

Significant Improvement of Thermoelectric properties of PbTe Nanocomposite system in the Medium-Low Temperature Range.

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By incorporating p-type micro- and nanostructured inclusions in the host PbTe nanocube matrix, electrical conductivity could be enhanced significantly due to an increase in hole carrier concentration. Importantly, the enhanced electrical conductivity was obtained without compromising the high Seebeck coefficient, which led to enhanced Power Factor. This 'decoupling' of Seebeck coefficient and electrical conductivity is due to energy filtering and tunnelling of charge carriers at the grain boundaries leading to optimized electronic transport. A high Figure of Merit (ZT) in the medium temperature range (approximately 550 K) were achieved in PbTe nanocomposite despite a small increase in its thermal conductivity highlighting the role of decoupled electrical conductivity and Seebeck coefficient due to the presence of micro- and nanostructured inclusions. Using PbTe nanocomposites as an example, we demonstrate a 10 fold enhancement in its thermo electric power factor through the incorporation of micro- and nanostructured inclusions that favorably modify the potential barrier height and width of its grain boundaries. Specifically, the tunnelling of charge carriers at the grain boundaries in (PbTe)_{0.89}(AgSbTe₂)_{0.1}(SnSe)_{0.01} nanocomposites along with the decoupling of its Seebeck coefficient and electrical conductivity due to energy filtering, lead to a ZT nearly 1.2-1.4 in the temperature range 450-550 K. This novel approach by which the barrier height and width of grain boundaries can be tuned favorably is attractive in our pursuit for high performance thermoelectrics.

Thursday, 22/Aug/2019 11:48am - 12:00pm

Abstract ID: 757 / FCM-3: 5

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Theoretical/Modelling/Computer Simulations Of Functional Materials

Keywords: Frozen-in magnetization, Magnetic fluid, Ultrasound, Anisotropy

Wave propagation in magnetic functional fluids

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Common types of magnetic functional fluid are magnetic fluid (MF) and magnetorheological fluid (MRF). The main difference between these two fluids is the inner particle size. The particles in an MF are about 10 nm in diameter, while those in an MRF are in the range 10 to 100 microns. The principal aim of the report is overview of the main results obtained in the framework of a new approach to the ferrohydrodynamics based on the concept of frozen-in magnetization. The condition of frozen-in magnetization leads to new equation of magnetization evolution. The discussion the connection the ferrohydrodynamics (FHD) with frozen-in magnetization with the existing theories is made in [1]. The FHD spectrum consists of three different waves: the Alfvén-type wave, the slow and fast magnetosonic waves [2]. Thus we have predicted existence of two new waves: the Alfvén-type wave and slow magnetosonic wave. The Alfvén-type wave in magnetic fluid similar Alfvén wave in perfectly conducting fluid. However Alfvén-type wave propagating in non-conducting magnetic fluid in an external magnetic field is accompanied by oscillations of the magnetization. From our point of view the experimental proof of existence of slow waves in MRF was received by Nahmad-Molinari et al [3]. We have described the experimental results [3] using the theory of wave propagation in magnetic fluid with frozen-in magnetization based on the linearized FHD equations. Also we have employed our theory to described the experimental data for the ultrasound velocity anisotropy in magnetic fluids based on the various liquids using the expression for the propagating velocity of the fast magnetosonic wave and good quantitative agreement between theory and experiment was demonstrated [2]. The prediction concerning the existence of the Alfvén-type waves in magnetic functional fluids seems very important and requires an experimental verification.

Key Words: Frozen-in magnetization, Magnetic fluid, Ultrasound, Anisotropy

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Abstract ID: 758

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Ferroelectric film

Keywords: Lead-free piezoelectric, epitaxial film, BNT-BT

Thickness-dependent phase transition and piezoelectricity in lead-free Bi_{0.5}Na_{0.5}TiO₃-BaTiO₃ epitaxial films

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Perovskite (1-x%)Bi_{0.5}Na_{0.5}TiO₃-x%BaTiO₃(BNT-BT_x) is one of the most promising candidates for lead-free piezoelectrics. The morphotropic phase boundary (MPB) at x=6, where the piezoelectricity reaches the maximum, separates a rhombohedral phase (x<6) and tetragonal phase (x>6). However, the MPB composition BNT-BT₆ is limited by the relative low depolarization temperature (T_d). On the other hand, the rhombohedral phase BNT-BT₂ has a high T_d but with a poor piezoelectricity. In this work, we investigated the phase structures and piezoelectric properties of the BNT-BT_x (x=2,6) epitaxial thin films with different thicknesses on Nb:SrTiO₃ substrates, attempting to construct a thickness-dependent phase boundary through stress control and to achieve an enhanced piezoelectricity at the phase boundary. Both BNT-BT₂ and BNT-BT₆ have smaller lattice parameters than that of the SrTiO₃ substrate. The reciprocal space mapping (RSM) results showed that both films suffered a tensile stress from the substrate and turned to a monoclinic phase at thickness<150nm, while further increasing thickness led to a stress release and the phase changed from monoclinic to the original state, rhombohedral phase. A maximum piezoelectric constant d_{33,eff}=60pm/V was achieved at the phase transition thickness ~150nm in BNT-BT₂. Such a thickness-dependent phase transition was also well demonstrated by the thickness-dependent domain evolution in piezoresponse force mapping (PFM) results.

Abstract ID: 759

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Nanomaterials for Sensors, Flexible Electronics and Nanocomposites

Keywords: Hydrothermal, β -Ag₂MoO₄ nanorods, diameter, NH₃ sensor

Selective sensing behaviour of 1D beta- Ag₂MoO₄ nanorods towards ammonia

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One dimensional nanomaterials received substantial attention for gas sensing applications due to their high surface area to volume ratio; tailored crystallinity and perfect pathway for electron transfer makes it a preferable choice over conventional bulk materials that comprised of randomly packed micro/nanoparticles. In particular, detection of ammonia in trace levels (TLV=25 ppm) is highly required to diagnose specific diseases and emissions from agriculture, animal husbandry, chemical industries, etc. Metal molybdates like β -Ag₂MoO₄ have received wide attention especially as a photosensitizer, photoluminescence, selective catalytic oxidation/reduction of NH₃/NO to N₂, etc. Herein, the selective response of β -Ag₂MoO₄ nanorods towards NH₃ has been achieved using the low-cost template-free hydrothermal technique. The systematic control of solution pH (HNO₃) facilitates the uniform growth of β -Ag₂MoO₄ nanorods. XRD pattern confirms the formation of the cubic phase of β -Ag₂MoO₄ and FE-SEM showed the uniform growth of nanorods with a diameter of ~80 nm and length of 2 - 4 μ m at pH 2 (Fig. 1). TEM micrograph of β -Ag₂MoO₄ also confirms the average diameter of 80 nm and SAED pattern reveals a single crystalline nature based on the well-defined diffraction spots recorded along the [-111] zone axis whose d-spacings agree well with the cubic phase of β -Ag₂MoO₄ (inset of Fig. 1). Nanorods of β -Ag₂MoO₄ exhibited selective response towards NH₃ among NO_x, H₂ and petroleum gas at 200°C. It is expected that the selectivity shown by β -Ag₂MoO₄ nanorods towards NH₃ (electron donor) is probably due to the electrophilic nature of chemisorbed O₂^-/O⁻, which are predominant species at 200°C. Moreover, when compared with conventional bulk materials, nanorods offered enhanced sensitivity to low concentrations of NH₃ (<5 ppm) with quick response and recovery times (<10 s) and with remarkable repeatability (Fig. 2). The salient outcomes of these experiments along with mechanism of sensing will be discussed.

Abstract ID: 760 / Poster: 17

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Biomaterials for soft tissue applications

Keywords: Electrospun nanofiber, tissue engineering, gene transfection

pDNA-activated Electrospun PLGA Nanofibrous Scaffolds for Tissue Engineering

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Electrospun nanofibrous scaffold is promising in tissue engineering due to its 2D and 3D fibrous structure which is analogues to the extra cellular matrix (ECM). They offer a number of key advantages including controllable fiber diameter, a huge surface area to volume ratio, a high porosity and permeability¹. Furthermore, these nanofibrous scaffolds can be “activated” by loading biochemical signals (e.g. proteins, genes) which will help to direct cell behavior². Herein, we developed pDNA (encoding Enhanced Green Fluorescent Protein (EGFP)-activated nanofibrous scaffolds by chemical grafting the fifth generation amino-terminated polyamidoamine (G5.NH₂) on biodegradable poly(lactic-co-glycolic acid) (PLGA) nanofibers and in situ gene compression. X-ray photoelectron spectroscopy (XPS) showed that N peaks were clearly observed on G5.NH₂-modified PLGA nanofibrous mats, indicating the successful grafting of G5. NH₂ on the nanofibers. Meanwhile, the surface roughness of PLGA nanofiber was greatly increased after grafting G5.NH₂ and the developed nanofibrous scaffolds exhibited improved hydrophilic property. Biological experiments showed that the developed system not only supported the attachment and growth of NIH 3T3 cells, but also able to transfect them with a transfection efficiency of 3.9% (Fig. 1), indicating the potential of developed nanofibrous scaffolds as effective gene delivery nanomaterials.

Figure 1. SEM images of (a) G5.NH₂-grafted PLGA nanofibers and (b) NIH 3T3 cells on G5.NH₂-grafted PLGA nanofibers, (c) Fluorescence microscopy image showing EGFP expression on G5.NH₂-grafted PLGA nanofibers 48 h post-transfection.

Thursday, 22/Aug/2019 8:42am - 8:54am

Abstract ID: 761 / FCM-2: 4

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Additive manufacturing Applications

Keywords: Lanthanum hexaboride, Additive Manufacturing, PA12, ATZ, Aluminum

Enhanced processing and material properties for powder based Additive Manufacturing with Lanthanum hexaboride composites

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Additive manufacturing (AM), the layer-by-layer production of parts from a wide variety of materials, is currently meeting great interest in science and industry [1]. Commercial machines for powder-based AM technologies typically work with a laser wavelength (λ) of 1.064 μm for metals (Selective Laser Melting (SLM)) and $\lambda = 10.6 \mu\text{m}$ for polymers (Laser Sintering (LS)). A material exchange between these two AM systems is not possible today. Materials such as polymers, oxide ceramics and some metals exhibit poor near infrared (NIR) absorption [2]. This low absorption makes it impossible to use SLM systems to process polymers and ceramic oxides. In addition, the processing of certain metals, such as aluminum, is difficult due to the high energy requirements. Lanthanum hexaboride (LaB6) nano-powder, on the other hand, shows considerable absorption in the near infrared range [3]. The aim of this work was to create a composite material with increased laser absorption that mixes LaB6 with AM powders that exhibit low NIR laser material interaction. Commercially available PA12 powder for LS (Duraform® PA), customized spray-dried aluminum oxide-zirconium oxide (ATZ) granules and commercially available aluminum alloys are homogeneously mixed with Nano-LaB6. All powders were processed on a SLM machine equipped with a standard Nd-YAG fiber laser (200 W, 1.064 μm). The parts were characterized in terms of density, mechanical properties and microstructure. It could be proven that PA12 and ATZ with $\lambda = 1.064 \mu\text{m}$ could be successfully processed. For example, Figure 1 shows six PA12 cubes processed with the Nd-YAG laser at ambient temperature resulting with a relative density of 97%. PA12 has mechanical properties comparable to the standard LS process, although the process is performed at room temperature. For the processing of LaB6 doped aluminum, a decrease in laser power compared to virgin material is expected. This work broadens the horizon of what SLM systems can do in terms of material processability.

Abstract ID: 762

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nanomaterials for Sensors, Flexible Electronics and Nanocomposites

Keywords: Fiber, Sensing Device, Energy Storage, Conductive Materials, Substrate

One- and Two-dimensional Fiber-based Sensing and Energy Storage Devices based on Conductive Materials and Yarn/Fabric Substrates

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One- and Two-dimensional Fiber-based Sensing and Energy Storage Devices based on Conductive Materials and Yarn/Fabric Substrates

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Fiber-based sensing and energy storage devices have attracted much attention as a next generation of flexible and wearable electronics. Compared to conventional metal- and film-based electronics, the fiber-based flexible and wearable devices have unique features, such as deformability, comfort, lightweight, washability and durability. In this talk, we report the recent progress on the development of one-dimensional yarn-based strain sensors based on a tri-coaxial architecture and the resultant two-dimensional fabric-based strain sensors by integrating the yarn sensing elements into the textile structures. The morphology and structure of sensors were examined by using scanning electron microscope and their mechanical and electro-mechanical properties were also evaluated based on a tensile and multimeter combined testing system. Besides, one-dimensional yarn-based flexible energy storage devices including supercapacitor and zinc-ion battery were fabricated by using the conductive yarn substrate and metal oxide materials for electrodes. Their electrochemical performance and stability were characterized. The experiment results show that such flexible and wearable fiber-based electronic devices have great potential for various applications in wearable electronics, robotics, medical diagnostics and healthcare.

Key Words: Fiber, Sensing Device, Energy Storage, Conductive Materials, Substrate

Acknowledgements

The work has been partially supported by the Research Grant Council of Hong Kong (Project PolyU 252024/16E) and The Hong Kong Polytechnic University (Project 1-ZE55).

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Abstract ID: 764 / Poster: 5

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Catalysis for pollution control

Keywords: Graphene, Sulfamethoxazole, Photodegradation

Application of N/S doping Graphene/TiO₂ on degradation of Sulfamethoxazole under visible irradiation

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Titanium dioxide (TiO₂) has emerged as a photocatalyst leader for environmental decontamination, however, the photocatalytic efficiency of TiO₂ is restricted under visible light irradiation because of the large intrinsic band gap (>3.2 eV) of TiO₂. A variety of strategies have been adopted to enhance the photocatalytic efficiency of TiO₂. The chemical modification of additional components in the TiO₂ structure is one of the most significant advancements [1-2]. In this study, a N/S doping rGraphene/TiO₂ was presented to investigate the degradation performance of sulfamethoxazole (SMX), one kind of antimicrobial agents, under visible irradiation of 410 nm.

The N/S doping rGO/TiO₂ were exhibited both anatase and rutile crystalline phase. The exhibition of rutile would extend characteristic adsorption wavelength to visible region. The characteristic absorption wavelength of N-doping and S-doping rGO/TiO₂ photocatalysts were shifted to 420-466 nm and 417-454 nm, respectively. The degradation of SMX by N-doping rGO/TiO₂ and S-doping rGO/TiO₂ under 410 nm irradiation was achieved to 10.7~59.0% and 5.2~40.6%, respectively. The degradation performance of N/S doping rGO/TiO₂ was dominated by graphene content, which showed the best degradation was found at 10% of graphene content. The formation of hydroxide radicals was also related to graphene content. The higher amount of hydroxide radicals produced would enhance better degradation of SMX. In this work, the degradation performance of N/S doping rGO/TiO₂ was dominated by graphene content. The hydroxyl radical (OH) was investigated and exhibited a significant relation to the SMX degradation.

Key Words: Graphene, Sulfamethoxazole, Photodegradation

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Abstract ID: 765

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Advances in Enzymatic and Non-Enzymatic Biosensors

Keywords: Label-Free Immunosensor, 3D Nanostructure, Graphene Oxide, Polypyrrole, Ionic Liquid

3D Label-Free Matrix Metalloproteinase-3 Immunosensor Based on Graphene Oxide/Polypyrrole-Ionic Liquid Nanocomposite

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Matrix metalloproteinase-3 (MMP-3) is a proteinase involved in the degradation of the extracellular matrix and it potentially plays an important role in metastasis development during the early stage of invasive cancers. In this work, a label-free electrochemical impedance immunosensor is for the first time developed for highly sensitive determination of MMP-3 based on the covalent immobilization of MMP-3 antibody on a 3D graphene oxide/polypyrrole-ionic liquid (GO/PPy-IL) composite film. The 3D GO/PPy-IL film was constructed by one step electro-deposition of GO/PPy in 1-Butyl-3-methylimidazolium tetrafluoroborate (BMIm+BF⁻⁴) onto a silica opal template modified indium tin oxide (ITO) electrode. Under the optimal conditions, the relative increased impedance values are proportional to the logarithmic value of MMP-3 concentrations in a linear range of 1 to 1000 pg• mL⁻¹ with a low detection limit of 1 pg• mL⁻¹. In comparison with current enzyme-linked immunosorbent assay, the MMP-3 immunosensor shows wider linear range, lower detection limit and simpler manipulation. Moreover, the immunosensor exhibits excellent selectivity, good stability, satisfactory reproducibility and regeneration. Such a 3D GO/PPy-IL film could have widespread applications in clinical screening of cancer biomarkers for point-of-care diagnosis.

Abstract ID: 766

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Thin films for optoelectronics, nanoelectronics and spintronics

Keywords: spin orbital coupling, surfaces, transitional metal oxides

The Inverse Rashba Edelstein Effect at the conducting SrTiO₃ surface

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The interface between oxides like LAO/STO has led to several emergent phenomenon such as superconductivity, magnetism and two dimensional electron gases. The spin orbital coupling arising from the asymmetric potential gives spin manipulation possibilities with a high efficient spin to charge current conversion. In this work, we show that this kind of conversion can also be obtained at surfaces.

The (001) surface of SrTiO₃ is transformed from insulating to conducting after Ar⁺ irradiation, producing a quasi two-dimensional electron gas (2DEG). This conducting surface layer can introduce Rashba spin orbital coupling due to the broken inversion symmetry normal to the plane. The spin splitting of such a surface has recently been demonstrated by magneto-resistance and angular resolved photoemission spectra measurements. Experimental evidence of a large spin-charge conversion at the surface is observed in this work. Spins are pumped from NiFe film into the surface of STO, and the resulting charge current is measured. The results indicate that the Rashba effect at the surface can be used for efficient charge-spin conversion, and the large efficiency is due to the multi-d-orbitals and surface corrugation. It holds great promise in oxide spintronics.

Abstract ID: 767

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nanomaterials for Sensors, Flexible Electronics and Nanocomposites

Keywords: Nanomaterials, I-V technique, Sensor

Legitimate Evaluation of Sensor Properties

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Legitimate Evaluation of Sensor Properties

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Sensors are continuously showing the promising applications as a sophisticated device in detecting the response of physical parameters such as humidity, temperature, pollutant, etc., in terms of electrical or optical signals. Sensing properties such as sensitivity, linearity, linear dynamic range, and slope of the linearly fitted curve, substantiate the signal response of electrode materials. Sensing properties of metal oxide nanoparticles based electrode sensors were explored through current versus voltage (I-V) technique. The value of the sensitivity is directly related to the value of the slope of the regression line, which is a function of the linear fitted curve within the selected dynamic range. Manual fitting of the linear curve within the selected dynamic range is tedious, factious, and portray the adverse effect on the value of the slope tailored/evaluated. Therefore, we are presenting a factual method to evaluate important sensor properties. A realistic approach to the evaluation of the sensor's properties is of great importance in identifying and differentiating the sensors for application purposes.

Abstract ID: 768

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Nanocomposites

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.

Key Words: Metal oxides, Activated carbon, Tyres, Nanofibers, Wastewater

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Abstract ID: 769

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Additive manufacturing Applications

Keywords: Nanocomposite, multi-functional materials, piezoelectric materials, additive manufacturing

Three-dimensional printing of piezoelectric materials with designed anisotropy and directional response

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Piezoelectric coefficients are constrained by the intrinsic crystal structure of the constituent material. Here we describe design and manufacturing routes to previously inaccessible classes of piezoelectric materials that have arbitrary piezoelectric coefficient tensors. Our scheme is based on the manipulation of electric displacement maps from families of structural cell patterns. We implement our designs by additively manufacturing free-form, perovskite-based piezoelectric nanocomposites with complex three-dimensional architectures. The resulting voltage response of the activated piezoelectric metamaterials at a given mode can be selectively suppressed, reversed or enhanced with applied stress. Additionally, these electromechanical metamaterials achieve high specific piezoelectric constants and tailorable flexibility using only a fraction of their parent materials. This strategy may be applied to create the next generation of intelligent infrastructure, able to perform a variety of structural and functional tasks, including simultaneous impact absorption and monitoring, three-dimensional pressure mapping and directionality detection.

Abstract ID: 770

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

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

Keywords: Memory Device, Organic Active Layer, Polysilicon Floating-Gate, SOI

Floating Gate Memory Device with Organic Active Layer Based on SOI Substrate

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Organic electronic devices have been considered to have great potential for the future electronic applications, among which the organic-semiconductor floating gate memories possess flexible structures, nondestructive read-out and easy implementation. We developed and characterized nano-structured floating gate memory devices. These devices were fabricated on SOI substrate, with organic semiconductor (p-type pentacene) as the active layer and polysilicon (poly-Si) as the floating gate. Different materials, such as SiO₂, Polystyrene (PS), Polymethyl methacrylate (PMMA) and Polyvinyl pyrrolidone (PVP), were used as the tunneling layer; the typical thickness was less than 10 nm. These devices present excellent storage characteristics in programming (P)-erasing (E) operation. The storage window is varying in a range of 10-20V, depending on the magnitude and time duration of the P-E stress and the material type of the tunneling layer. The P-E loops of these devices are of electrical hysteresis, indicating that the poly-Si floating gate is capable of capturing both electrons and holes. The required P-E stressing bias can be effectively reduced by changing the material and optimizing the thickness of the tunneling layer. Devices with SiO₂ and PS tunneling layer are uniformly superior to those with PMMA and PVP in transfer characteristics and programming-erasing performance. Detailed investigations show that there exists optimum matching between the the tunneling layer and active layer in terms of material and geometrical parameters, which need to be modified to achieve optimal performance.

Wednesday, 21/Aug/2019 6:54pm - 7:09pm

Abstract ID: 771 / FBB-2: 15

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Plenary

Topics: Microfluidics

Keywords: Compound channel, Impactor, Microfluidic, Stokes number

Performance Evaluation of Particle Separation Impactor with an Additional Compound Structure

Pan Wang, Ning Yang, Shouqi Yuan

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In this study, to improve the collection efficiency of specific particles, a novel compound microfluidic channel was designed before the impactor, which can arrange the particles according their particle size by generating the sheath flow and backward-facing step flow. To verify the compound structure effects, simulations and experiments were conducted. Basic parametric studies were performed on the proposed separator to improve the collection efficiency and modify the collection curve based on PM2.5 virtual impactor. As a result, the performances including the cut-off size and wall loss (WL) were examined by classifying Sodium chloride (NaCl) of 0.5 to 4 μm in size. The cut-off size was reduced by 26.4 % from 2.5 μm to 1.84 μm and the rate of WL was reduced significantly compared with only using one impactor. The improvement of efficiency could be observed even when Reynolds number varies. Accordingly, the stk_{50} value was reduced by 70.76% from 0.667 to 0.195 by adding an additional pretreatment in a virtual impactor. In addition, the effect of the novel method on PM1 and PM5 was also investigated.

Abstract ID: 772 / Poster: 6

**Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)
Poster Presentation**

Topics: Nano-optics, Nano-optoelectronics, Nano-Photonics and Nano-photonics

Keywords: disordered, nanostructure, random laser

Reobservation of GaN Nanostructures for Random Laser

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Unlike a conventional laser, random laser has the scattering medium in which itself serves as virtual cavity and emits the light in different directions. Recently, scattering medium of random laser has been designed such as photonic crystals, quantum dots, and semiconductor.[1] Randomly distributed nanostructures have the potential to be used as scattering medium of random laser. As mechanism of light localization for random laser is scattering in gain medium, one of the main factors of random lasing is density of nanostructures.[2] Here, we fabricate GaN nanostructures, as shown in Figure 1, via tunable density of disordered SiO₂ mask. First, we grow SiO₂ on GaN on sapphire substrate via plasma enhanced chemical vapor deposition and Ag using electron beam evaporator. After that, we process thermal dewetting of Ag for etching mask, and dry etching of SiO₂ by reactive ion etching, and Ag removal via HNO₃ solution. Finally, we implement GaN nanostructures by inductively coupled plasma reactive ion etching with SiO₂ mask and buffered oxide etchant for SiO₂ removal. We show various density of GaN nanostructures which exhibit the different number of lasing mode. Further, we inspect the tendency of random laser phenomenon by line scanning. With this spatial scanning, we can exhibit spatial characteristic of random lasing, which show the probability of random lasing intensity above the threshold is governed by Poisson distribution.

Key Words: Disordered, Nanostructure, Random laser

Acknowledgments

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Wednesday, 21/Aug/2019 4:15pm - 4:27pm

Abstract ID: 773 / FC: 2

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalysis for pollution control

Keywords: Amorphous alloy, Zero valent iron, Degradation efficiency, Oao dye

Fe-based amorphous/nanocrystalline alloys with high efficiency in degradation of oze-dye containing wastewater

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Amorphous alloys, possessing a unique structure of long term random packing of atoms, are a kind of metastable materials and occupying higher energy level than their crystalline counterpart in thermodynamics. Amorphous alloys usually contain more constituents, making them possess relatively high entropy in alloys. In contrast with their crystalline counterparts, due to lack of defects like grain boundaries or interphase boundary and the difference in crystalline orientation, amorphous alloys are chemical homogeneity, which ensure the chemical reaction occurs all over the surface without preference. As a result, the unique structure endows amorphous alloys many special properties. Recently, it has been found that iron based amorphous alloys could exhibit higher degradation efficiency than crystalline zero valent iron (ZVI), which has been widely studied to reductively decompose a series of oxidative hazardous materials like chlorinated pesticide, azo dyes and so on since 1980s.

In our group, the degradation behaviours of azo dyes with Fe-based metallic amorphous ribbons, which are recognised as amorphous zero valent iron (AZVI), and the related mechanism have been studied. It has been found that Fe-based amorphous ribbons exhibit much higher degradation efficiency than their crystalline counterparts and commercial 300 mesh iron powders despite of that the specific surface area of AZVI ribbons is much smaller than that of ZVI powders. The Fe-based amorphous ribbons possess low reaction activation energy in degradation of azo dyes. But the degradation mechanism of the Fe-based amorphous alloys is the same as that of crystalline ZVI. The higher degradation efficiency of the amorphous alloys ribbons is attributed to the amorphous structure, the thermal dynamical status, the chemical homogeneity and the difference in the composition. The large number of reactive sites, which is ascribed to the chemical homogeneity, is the most significant factor. The present results indicate that Fe-based amorphous ribbons are high performance materials in degradation of azo dyes and could be applied as new ZVI materials for rapid decomposing organic pollutants.

Abstract ID: 774

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Microfluidics

Keywords: cell signaling, DNA origami, microfluidics

Origami-based Microfluidic Interface for Cell Signaling

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We present here a microfluidic device for the investigation of early cell signaling, which is triggered by ligand-decorated DNA origami nanostructures, immobilized on a microarray-patterned surface inside the microfluidic device. By combining state-of-the-art top-down microstructuring and bottom-up self-assembly of DNA origami structures, this approach allows to present ligands on surfaces with a full control of their absolute number, stoichiometry and nanoscale orientation. The implementation of origami-based ligand presentation in a microfluidic chip improves the surface stability and robustness, and allows automated on-surface assembly and cell culture processes, paving the way to multiplexing and high throughput analyses.

Abstract ID: 775

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Synthetic biomaterials

Keywords: Silica nanoparticles, carbon nanotubes, DNA, nanocomposites, rolling circle amplification

Carbon-Nanotube Reinforcement of DNA-Silica Nanocomposites Yields Programmable, Cell-Instructive Biocoatings

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Biomedical applications require substrata that allow for the grafting, colonisation and control of eukaryotic cells. Currently available materials are often limited by insufficient possibilities for the integration of biological functions and means for tuning the mechanical properties. To overcome these limitations, we have developed tailorable nanocomposite materials in which silica nanoparticles are interwoven with carbon nanotubes by DNA polymerization. The modular, well controllable and scalable synthesis yields materials whose composition can be gradually adjusted to produce synergistic, non-linear mechanical strength and viscosity properties. The materials were exploited as novel substrata that outperform conventional culture surfaces in the ability to control cellular adhesion, proliferation and transmigration through the hydrogel matrix. The composites were also applied for expansion of embryonic stem cells by simplified cultivation procedures. Furthermore, incorporation of enzymatic restriction sites into the polymeric DNA backbone enables control of transmigration to construct layered cell architectures and to achieve on-demand release of cells in static and fluidic culture systems. All approaches demonstrate high biocompatibility and adjustable cell-surface interactions. Since materials libraries can be readily constructed, via automated synthesis, the novel composites provide a platform with high potential for fundamental studies and device applications in biomedical sciences.

Abstract ID: 776

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Biomaterials for Cardiovascular Applications

Keywords: Nitric oxide, polycaprolactone), small diameter vascular grafts, electrospinning

In-vitro and in-vivo evaluation of small-diameter nitric oxide-eluting biodegradable vascular grafts

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Objective: Synthetic small diameter vascular grafts reveal low patency rates because of thrombus formation and intimal hyperplasia development. Bio-functionalized conduits which release in-situ nitric oxide (NO) may overcome these limitations because NO has crucial roles in the regulation of thrombus formation, endothelialization and intimal hyperplasia. Here, we aimed to design a bioactive vascular graft by physical blending polycaprolactone (PCL) with a previously patented highly stable NO donor.

Material and Methods: PCL conduits blended with s-nitroso human serum albumin (S-NO-HAS) were fabricated by electrospinning and characterized in-vitro (NO-release, biomechanics, inflammatory effects and cell proliferation). Grafts were further evaluated in a small rodent model as aortic implants (2 weeks, 1, 3 months, n=21). Non-modified grafts were used as controls (n=21). Grafts were assessed by MR angiography in-vivo and after retrieval by histology and biomechanical analysis.

Results: S-NO-HAS loaded grafts revealed significantly enhanced endothelial cell proliferation in-vitro while smooth muscle cell proliferation was significantly decreased. S-NO-HAS attenuated the expression of ICAM-1, VCAM-1 and TF and up-regulated anti-inflammatory cytokines (IL10) and M2 macrophage marker (CD163), whereas pro-inflammatory markers (CD80, IL1 α , TNF α) were significantly down-regulated. The patency rate of all grafts was 100 %. S-NO-HAS loaded grafts showed superior endothelialization compared to non-loaded grafts. Cell migration into the graft wall differed significantly between S-NO-HAS-PCL- and PCL-conduits.

Conclusion: These data indicate that S-NO-HAS-PCL grafts support long-term in-situ release of bioactive NO with promoting effects on graft endothelialization. However, the desired suppressive effect of NO on smooth muscle cells to prevent intimal hyperplasia lead to limited cell migration into the graft wall. Therefore the application of S-NO-HAS is only appropriate for non-resorbable grafts which do not require essential scaffold remodeling.

Keywords: Nitric oxide, poly (ϵ -caprolactone), small diameter vascular grafts, electrospinning

Abstract ID: 777

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Spectroscopy studies of low dimensional, nano and 2D materials Carbon Based materials

Keywords: Tin(II) monosulfide, Phonon dynamics, Exciton-exciton annihilation

Exciton and phonon dynamics in two-dimensional tin(II) monosulfide

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Phosphorene, a monolayer of black phosphorus (BP) has sparked a surge of research activities in material science since first exfoliation. The strong structural anisotropy is the origin of its unique in-plane anisotropic electrical, optical, and mechanical properties, which are different from conventional isotropic two-dimensional (2D) semiconductors. But, it has the drawback of rapid degradation in ambient condition. Recently, earth-abundant 2D tin(II) monosulfide (SnS) with more environmental stability has emerged as an analog of phosphorene. However, the preparation of thinner SnS sheets having larger lateral dimension is challenging. We exfoliated thinner (as thin as bi-layer) 2D SnS of much bigger size (six-layer ~ 20 micro-m, four-layer ~ 5 micro-m and bi-layer ~ 160 nm) through liquid phase exfoliation technique. Temperature dependent Raman spectroscopy, transient absorption spectroscopy and Z-scan techniques were employed to investigate the electron-phonon and exciton-exciton interactions in 2D layered SnS. Our results reveal that bi-layer SnS exhibits a linear phonon dynamics, while nonlinear behavior is dominant in few-layer SnS. Raman modes of 2D SnS exhibit more sensitivity to temperature than other 2D materials. Ultrathin SnS possesses strong nonlinear optical behavior leading to saturable absorption. The strong Coulomb interactions in 2D SnS give rise to exciton-exciton annihilation (EEA) at low excitation density leading to quick decay of the exciton population. But, at higher exciton intensity, hot exciton is formed via Auger process. A biexciton is finally formed from hot exciton through absorption of another photon of low energy. The strong many-body interactions in turn enhance nonlinear optical response of 2D SnS by making them potential candidates for photonic applications. This study highlights the nature of the phonon and exciton dynamics in anisotropic 2D SnS for futuristic thermoelectric and photonic device applications.

Key Words: Tin(II) monosulfide, Phonon dynamics, Exciton-exciton annihilation

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Abstract ID: 778

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: Nanocomposite, Piezoelectric, Energy Harvesting

Deformation induced energy generation using 0.5(Ba_{0.7}Ca_{0.3})TiO₃-0.5Ba(Zr_{0.2}Ti_{0.8})O₃/PVDF nanocomposites

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Recently, considerable attention has been given on the ceramic/polymer composites due to the growing demands in electronic and/or microelectronic industries for the development of multifunctional devices and trend towards miniaturization. They have got a wide range of technological applications such as in embedded passive technology, high-speed ICs, high charge storage capacitors, gate dielectrics, sensors, actuators, energy harvesting, artificial muscles, smart skins, etc. [1]. In recent years, large numbers of polymer-based 0-3 composites with non-lead ceramics as fillers have been studied with different aims [2]. It is known that the piezoelectric materials with Perovskite ABO₃-type structure, under impact loading undergoes deformation and causes oscillations of dipoles within them which give rise electric voltage. Accordingly, results of 0.5(Ba_{0.7}Ca_{0.3})TiO₃-0.5Ba(Zr_{0.2}Ti_{0.8})O₃/poly(vinylidene fluoride) nanocomposites in 0-3 connectivity under the impact loading will be presented. These ceramic/polymer nanocomposites have been prepared using melt mixing method which was characterized using XRD, SEM, AFM-PFM, dielectric, impedance and piezoelectric (d₃₃) studies for their possibility to be used for piezo-sensing and/or energy harvesting applications.

Key Words: Nanocomposite, Piezoelectric, Energy Harvesting

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Abstract ID: 779

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: MoS₂/Ag, MoS₂/ZnO, Nanocomposites, Photocatalysis

MoS₂ based nanocomposites for photocatalytic degradation of industrial dyes

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Textile industries produce one of the major contributors to industrial effluents i.e. dyes. These dyes are deadly for marine life and environment. To maintain ecological balance, degradation of these noxious dyes to environment friendly compounds is need of the time. A suitable and efficient photocatalyst make photocatalysis a promising approach for this purpose. Molybdenum disulphide (MoS₂) possess unique properties such as direct band gap and sandwich molecular layered structure which makes it suitable as photocatalyst. However, MoS₂ have active sites for photocatalytic applications but lack of emission sites, high electron-hole recombination and stacking faults limits its use. To overcome these limitations, MoS₂ based nanocomposites (MoS₂/ZnO and MoS₂/Ag) has been synthesized in this work. X-ray diffraction analysis confirmed the formation of nanocomposites. Nelson Riley factor calculation showed the presence of defect states which plays an important role in photocatalytic mechanism. The as synthesized nanocomposites have been used for the degradation of Novacron red huntsman (NRH) dye. MoS₂/Ag (30%) photocatalyst with 1g/L concentration results in ~78% degradation whereas MoS₂/ZnO (30%) leads to 81% photodegradation of NRH within 80 minutes. Improvement of photocatalytic activity can be ascribed to particle size, structural defects, morphology and presence of more active sites. These results make MoS₂ based nanocomposites a favorable photocatalyst for degradation of industrial pollutants.

Abstract ID: 780

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nanomaterials for Energy and Environmental Applications

Keywords: Nanocomposites; PbTe; Single Wall Carbon Nanotubes; Thermoelectric

Thermoelectric properties of Lead Telluride (PbTe) based single wall carbon nanotube (SWCNT) composites

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Thermoelectrics have long been recognized as a promising energy conversion technology due to their ability to convert waste/solar heat into electricity. There are continued efforts to improve their low efficiency for broader applications. Recently, incorporation of low dimensional constituents such as single wall carbon nanotubes (SWCNTs) through nanostructured powder processing has evolved as a cost effective and scalable strategy for the development of high performance thermoelectric bulk materials [1, 2]. The focus of the present work is to enhance energy conversion efficiency of PbTe by mixing SWCNTs via facile powder processing through synergistically utilizing the nanostructuring and quantum confinement effects. In a simple and effective strategy we were able to demonstrate different vol% of SWCNTs ranging from 0.5, 0.75, 1.0 and 1.5 were uniformly dispersed in fine powder of PbTe that was ball milled from coarse PbTe in an inert environment. The coarse PbTe and fine composite powders were consolidated in a high frequency induction heated sintering furnace at $\sim 400^{\circ}\text{C}$ under uniaxial pressure of ~ 40 MPa. Thermoelectric properties of PbTe based SWCNTs bulk samples were evaluated in the temperature range from ~ 300 to $\sim 530\text{K}$. The results suggest that electrical conductivity behavior transforms from semi-metallic in pristine PbTe to semi-conducting in the composites with the addition of nanotubes. This indicates that electrical transport dominantly involves semiconducting nature of SWCNTs. Consequently, the effective electrical conductivities of the composites suppressed near room temperature from the pristine PbTe and lowest values were observed at 0.5 vol% of SWCNTs. Accordingly the Seebeck coefficient at 0.5 vol% PbTe composite improves near room temperature from pristine bulk while above ~ 375 K it decreases gradually. Thermal conductivity of all the composites decreases with the addition of SWCNTs and substantial reduction was achieved at 0.5 vol% attributed to enhanced phonon scattering through uniform distribution of nanotubes. The results suggest that major shift from semi-metallic transport in pristine bulk to semi-conducting in the composites as well as increased short range carrier scattering possibly contribute in suppressing of electrical conductivity that leads to decrease in power factor of all the composites. Hence, the considerable reduction in thermal conductivities could not compensate for lessening in power factor and consequently lower values of ZT were observed in the composites from pristine PbTe bulk. The metallic nature of SWCNTs with enhanced densification could improve energy conversion efficiency of PbTe.

Abstract ID: 781

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Nanomaterials for Biomedical Applications

Keywords: Cashew nut shell liquid, Nanostuctured, Antibacterial

Agro byproduct derived functional materials: Synthesis and characterizations

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In the present work, reports the development of micro to nanomaterials from an agro byproduct of cashew industry (cashew nut shell liquid) to evaluate their potential in antibacterial applications as an alternative to substitute petroleum feedstock. The synthesis of agro byproduct derived micro to nanostructure functional materials were carried out by applying the principles of “Green” Chemistry. Synthesized functional materials were characterized by different standard techniques. FTIR and ATR was used to confirm the proposed structure and curing of the material. Morphology of the materials was investigated by XRD, SEM and TEM, while thermal stability investigated by TGA. Antibacterial activity of these materials were evaluated by agar diffusion methods against different gram positive and negative strains. These results finding reveal that the synthesized functional materials obtained as amorphous/semicrystalline and nanostructured film forming materials along with moderate to good antibacterial activity against different nosocomial bacteria. These functional materials can be used as antibacterial agents in the field of antibacterial films/coatings for health care applications.

Abstract ID: 782

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Anti-cancer therapy

Keywords: Nanostructures, B₄C, Cytotoxicity, BNCT

Nanostructured boron carbide for cancer treatment by boron neutron capture therapy

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Malignant tumors are the leading target of boron neutron capture therapy (BNCT). This technique is a boon for tumors where surgery is very complex or not possible. It requires a proper choice of neutron source and boron source (¹⁰B isotope) to achieve better results. Nowadays, boronophenylalanine (BPA) and sodium borocaptate (BSH) are two clinically used boron compounds in BNCT. But in some cases, these compounds lack in various aspects. Research on new boron based compounds, especially nanostructured materials, is extensive these days. But difficult synthesis route, degradation into toxic products and presence of less amount of boron are some hurdles in the development of new boron based material. Present work deals with the synthesis, cytotoxicity and BNCT studies of nanostructured boron carbide (B₄C). This compound can be easily synthesized by a single step process using solvothermal route and is very stable even at high temperature. Structural and morphological analysis confirms the formation of nanostructured boron carbide with average particle size ~15-20nm. Cytotoxicity studies on normal and cancerous cells showed that B₄C can be used in biomedical applications as these nanostructures are relatively less toxic at lower doses. BNCT studies were performed using thermal neutron source at Kyoto University Research Reactor, Japan. BNCT of boron carbide on HeLa cells was performed in comparison to BPA. The anti-tumor effect of nanostructured boron carbide showed positive and similar results to the clinically studied compound. Hence, B₄C can be a promising direct boron compound for the treatment of malignant tumors using BNCT.

Abstract ID: 783 / Poster: 22

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Biomaterials for hard tissue applications

Keywords: Decellularized Bone Matrix, Magnetic Biomaterials, Tissue Engineering

Magneto-Sensitive Decellularized Bone Matrix as a Regenerative Biomaterial

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Matrix-based products derived through the decellularization of natural tissues are increasingly used in regenerative medicine applications. Decellularized bone matrix (DBM) is rich in growth factors, hormones, proteoglycans, and induces cell adhesion, migration and differentiation. DBM has brought a new perspective to the bone regeneration concept; however, it is usually prepared in powder form and delivered into the bone defects in combination with polymers. The versatility of such products affects its regenerative properties. We have developed a magneto-sensitive bone matrix-based composite biomaterial by decellularizing natural bone tissue with chemical and enzymatic processes and then combining with superparamagnetic iron oxide nanoparticles (SPIONs) obtained by the precipitation method. Our optimized decellularization process efficiently reduces the nucleic acid content, while preserving significant amount of the bioactive components of the bone tissue. Magneto-sensitive DBM is hemocompatible as confirmed by the in-vitro biocompatibility analysis. Combination of DBM with SPIONs improves the mechanical properties of the DBM while also allowing the biomaterial to be sensitive to magnetic fields which can be applied from outside of the body, thus increasing the regenerative activity in-vivo.

This study is financially supported by TUBITAK (216S575).

Abstract ID: 784

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Invited Talk

Topics: Synthesis, Controllable Growth and Characterizations

Keywords: Schiff base, Coordination Complex, Antibacterial

Schiff base derived coordination complexes / polymeric materials for biological applications

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The development of new complexes/polymeric advanced functional materials is a demand of polymer chemistry and technology for biologically applications. Coordination complexes/polymers have gained great attention in this field and found tailormade applications. They have been prepared by complexation of monomeric / polymeric ligands with metal ions. The nature of these functional materials depend not only on metal ions but also on the structure of the ligands and the metal–ligand interactions. Multidentate amines, crown ethers, porphyrins, macrocycles and Schiff bases have been widely used as organic linker or ligand for coordination complexes/polymers. Among them Schiff base {or imine (N=CH-) linkags} has gained much attention due to their good thermal stability, useful mechanical properties, flexibility, structural similarities with natural biological substances. The complexation of Schiff bases with metal ions with not only affects their physical characteristics, but also their chemical activity. Schiff bases could also act as valuable ligands whose biological activity has been shown to increase on complexation. The present work reports new Schiff base monomeric or polymeric ligands (with N, O or S) and transition metal ions based functional materials for their application as biologically active reagents. They have been characterized by spectral techniques (IR, ¹H-NMR and UV-visible). The elemental analysis, magnetic moment measurement and thermal behaviour of these materials along with geometry of the central metal ions have also been discussed. They have been screened for their biocidal activity against different microbes by agar well diffusion method. These studies reveal that the geometry of these materials changes with the complexion of transition metal ions. Amongst them Cu (II) ions based materials show higher antimicrobial activity and thermal stability than the others and virgin ligands. The synthesized function materials can be used as antibacterial agents.

Abstract ID: 785

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: Epoxy matrix, nano composites, DGEBA epoxy resin, nano CaCO₃.

Thermal, Mechanical and Chemical Characterization of Nano Composites Prepared from DGEBA Epoxy Matrix and Nano CaCO₃

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Advancements in nano technology industries promise to offer improvement in capabilities across the spectra of applications of polymeric matrices. The numbers of thermoplastic and thermosetting matrices are subjected to improve the various properties like mechanical strength, thermal stability and chemical resistance via incorporation of nano fillers. The epoxy resin matrices are most commonly used for thermosetting resin matrix used for a number of applications such as coatings, floorings, electrical and electronics applications, adhesives, non conducting materials and encapsulations due to their excellent mechanical and thermal properties [1-2]. But, it becomes brittle when cured, restrict to a number of engineering applications due to poor mechanical and thermal properties [3-4]. The studies showed that the addition of nano size fillers in the epoxy resin matrix can drastically enhance the mechanical properties, thermal stability and chemical resistance of the matrix.

In the present study Epoxy/CaCO₃ nano composites were prepared by mechanical mixing of DGEBA epoxy resin having epoxide equivalent weight (EEW) 180 g/eq and varying concentrations of nano CaCO₃ ranging between 1-10 wt% followed by sonication for 30 min. The prepared Epoxy/nano CaCO₃ mixtures were poured into the Teflon mold and subjected to curing at 110°C for 1 hour and post curing at 80°C for 5 hrs. The prepared nano composite samples were investigated for the mechanical properties (viz. The tensile strength, elongation at break, impact strength and modulus), thermal stability and chemical resistance properties of nano composite samples. It was observed that the mechanical properties, thermal stability and chemical resistance increased as the nano filler concentration increased in samples. It was observed that the maximum values of all three properties were found in 5wt% nano CaCO₃ loaded sample. It was observed that the sample containing 5 wt% nano CaCO₃ in epoxy matrix showed maximum thermal stability as compared to other compositions of nano composite and neat epoxy matrix. The prepared samples were also investigated for the non reactivity of nano filler towards resin matrix by FTIR spectroscopic analysis, morphology by SEM and curing studies by DSC.

Key words: Epoxy matrix, nano composites, DGEBA epoxy resin, nano CaCO₃.

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Abstract ID: 786

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Fiber reinforced Composites

Keywords: Carbon fibers, copper composites; electroless deposition; powder metallurgy; electrical resistivity.

Microstructure and Properties of Carbon Short Fibers/Copper Composites Fabricated by Electroless Deposition Followed by Powder Metallurgy Technique

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Carbon short fibers/copper metal matrix composites with different carbon short fibers contents up to 15wt.% as reinforcements are prepared to investigate the influence of the carbon short fibers surface coating on the microstructure, density and electrical properties of the sintered composites. The carbon short fibers were surface treated and metallized by silver deposition. It was observed from the results that decorated type silver nanoparticles were deposited on the surface of the carbon short fibers. The silver metallized carbon short fibers were coated by copper using the electroless deposition technique in the alkaline tartrate bath using formaldehyde as a reducing agent of the copper sulphate. The produced coated carbon short fibers/ copper composite powders were cold compacted at 600 MPa, and then sintered at 875°C for 2 h under (hydrogen/Nitrogen 1:3) atmosphere. A reference copper sample was also prepared by the same method to compare between the properties of pure copper and the sintered composites. The phase composition, morphology and microstructure of the prepared carbon short fibers/copper composite powders as well as the corresponding sintered copper composites were investigated using X-ray diffraction analysis (XRD) and Scanning Electron Microscope (SEM) equipped with an Energy Dispersive Spectrometer (EDS) respectively. The density and the electrical resistivity of the sintered composites were measured. It was observed from the results that; the density was decreased however the electrical resistivity was increased by increasing the carbon short fibers wt. %.

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Thursday, 22/Aug/2019 8:54am - 9:06am

Abstract ID: 787 / FCM-2: 5

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Dielectric, Ferroelectric and Piezoelectric materials

Keywords: Interpenetrating phase piezoelectric composite, infiltration processing, infiltration kinetics, poroelasticity, piezoelectricity

Modeling of Infiltration Processing of Interpenetrating Piezoelectric Composites

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This work presents a poro-piezoelectricity model to investigate isothermal infiltration of a porous piezoelectric ceramic by a Newtonian fluid. Governing equations for fluid-infiltrated porous piezoelectric materials are first formulated based on the theories of poroelasticity and piezoelectricity. A similarity solution is obtained for infiltration of a piezoelectric ceramic under one-dimensional strain and flow conditions. A numerical example for infiltration of a PZT by a liquid polymer indicates that the infiltration kinetics and pore fluid pressure are insensitive to the piezoelectric constant of the material. The fluid content variation, however, strongly depends on the piezoelectric and dielectric constants of the piezoelectric ceramic preform.

Abstract ID: 788

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: Boron Nitride, Nanocomposites

Boron nitride nanomaterials modifications to improve nanocomposites preparation

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The unique multifunctional properties of boron nitride (BN) nanomaterials are identified as a parameter that would revolutionize electric propulsion in Aeronautics. Having BN as a part of ceramic or polymer composites can improve the matrix properties by simultaneously achieving high thermal conductivity and low electrical conductivity, along with high mechanical strength, low weight and chemical inertness. These materials properties are essential for components used in high voltage electric system of electric or hybrid electric airplanes. However, synthesis and processing of these BN-modified composites has proven to be difficult because the chemical inertness and thermal stability of BN prevent filler matrix bonding. Our research team has demonstrated significant improvements in composite processing while using hexagonal BN (hBN) as a filler, using intercalation, exfoliation, coating and/or chemical functionalization of hBN. Functionalization of h-BN by oxidation and subsequent chemical bonding of polymer helped to improve dispersion for polymer composites. On the other hand, intercalation, exfoliation and coating of hBN with other ceramic matrix materials resulted in decreasing of the temperature required to hot-press the ceramic composites. In spite of the team accomplishments, there are still many areas for improvement remain in development of composite materials with properties tailored to different aeronautics applications. This presentation will demonstrate a summary of mechanical, thermal and electrical properties of hBN-modified materials, with prepared composites being evaluated by FTIR, SEM, XRD and thermal conductivity measurement techniques.

Abstract ID: 789

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Additive manufacturing Applications

Keywords: Sensors, Polymer-matrix composites (PMCs), Additive manufacturing, Multifunctional materials

3D printed CNT and continuous fiber reinforced hybrid composite for multifunctional applications

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Fused filament fabrication (FFF)-based additive manufacturing (AM) of polymers and composites is a growing interest in processing smart, multifunctional materials in a tailorable paradigm. The state-of-the-art of FFF process is the continuous-fiber reinforced polymers (CFRP). However, the technology must provide end-user products with sufficient mechanical integrity and multifunctional capabilities for sustainability. The continuous fiber reinforced-AM approach brings out a new scope for multifunctional applications by entailing not only the seamless integration of dissimilar materials but also the embedding of active components in order to offer functionality. Such advancement can potentially combine chemical, thermal, electronic, electromagnetic, acoustic, and optical features into printed components including sensing, thermal management, structural health monitoring, and electromagnetic utilities.

This paper is focused on understanding the underlying physics behind the FFF of continuous fiber reinforced hybrid composites through a detailed microstructure analysis, characterization of mechanical and electrical properties of 3D printed hybrid nanocomposites. Different material layers will be customized in FFF-CFRP depending on the functional requirements. For example, the structural strength and stiffness can be enhanced incorporating continuous carbon fiber in the critical stress concentration areas. The high strain Kevlar fiber is capable of offering both strength and high impact sensing capability. The electrically conductive carbon nanotube reinforced nylon can be used as the resin material offering good electrical conductivity as well as fiber-matrix bonding. Moreover, it is possible to tailor the orientation of both the CNTs and continuous fibers which adds extra dimension over the functional requirements. The proposed architecture can be used in many applications such as aircraft where the continuous fibers can support the load, CNT-nylon matrix can work as pressure and strain sensors.

Unidirectional tension test coupons of hybrid CNT/nylon-carbon-Kevlar composite will be fabricated using FFF-AM and tested for characterizing the mechanical properties. The electrically conductive CNT-nylon nanocomposite matrix will be prepared in-house using laboratory extruder. Proper surface treatment will be introduced to improve the dissimilar fiber-matrix interfacial interaction and the surface characterization will be performed through Fourier-transform infrared (FTIR) spectroscopy. The fiber dispersion and distribution in the matrix will be investigated through optical and scanning electron microscopy.

Wednesday, 21/Aug/2019 5:12pm - 5:24pm

Abstract ID: 790 / FBB-2: 7

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Engineering of tissues and regenerative medicine

Keywords: Diabetes Mellitus, Nano, Polypyrrole Plasma, Pancreatic Islets, Encapsulation.

Polypyrrole nanoparticles synthesized by plasma as promoters of rat pancreatic islets capsules

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Type 1 diabetes mellitus is a disease associated with a total insulin deficiency. In last decades it has been reported that the transplantation of pancreatic islets in humans and different types of biological models with type 1 diabetes mellitus, restored the normal blood glucose levels. However, pancreatic islets are destroyed by the host immune response, for this reason, different types of biomaterials have been developed to encapsulate and protect them from the host immune response. These biomaterials must keep alive the pancreatic islet cells and allow the release of insulin. It has also been reported that the polypyrrole synthesized by plasma is a biomaterial that has good cell adhesion, improving the viability and functionality of different cell types, also showing neuroprotective effects and decreasing the inflammatory response in spinal cord injury in rats. We covered rat pancreatic islets with polypyrrole nanoparticles synthesized by plasma (NPPP) to develop a capsule that protects the pancreatic islets of the immune system. The scanning electron microscopy images showed that the NPPPs have spherical morphology, the diameter distribution of the NPPP had a normal distribution with a mean of 488 nm and a standard deviation of 70 nm. The infrared spectrum showed that the NPPP structure has a strong presence of hydroxyl groups and primary amines. The rat pancreatic islets were observed with an optical microscope, the size and morphology of the pancreatic islets were similar to those reported by other authors. The secretion of insulin from the pancreatic islets was measured during the first five days of culture, reaching a maximum on the third day of culture and beginning to decrease during the following days. Pancreatic islets were successfully covered with NPPP, the NPPP improved the viability of pancreatic islets and the encapsulation was evaluated by culturing mouse splenic lymphocytes with rat pancreatic islets covered with NPPP. This study offers a promising exploration of the polypyrrole synthesized by plasma as a biomaterial for the encapsulation of rat pancreatic islets that may have an important application as a treatment for type 1 diabetes mellitus.

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Thursday, 22/Aug/2019 8:24am - 8:36am

Abstract ID: 791 / FLNM: 3

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Synthesis, Controllable Growth and Characterizations

Keywords: Graphene template, Anisotropic, Surfactant-free, Au nanocrystals

Graphene-Templated Growth of Surfactant-free Anisotropic Gold Nanocrystals

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Gold nanocrystals with isotropic structures, e.g. nanoparticles in the spherical shape, are thermodynamically favorable and stable. To obtain anisotropic Au nanocrystals in a wet chemistry synthesis, surfactants or capping agents are indispensable, which passivate the nanocrystals and cause removal issues for their following applications.¹⁻³ Here, we report surfactant-free synthesis of a variety of anisotropic Au nanocrystals with the direction of graphene template under appropriate conditions. We observe these gold nanocrystals are all single-crystalline, including Au nanowires, Au nanoribbons, and Au nanobelts. The role of graphene template playing in these syntheses is systematically investigated. We reveal that graphene serves as the reductant for gold precursor that reduces Au³⁺ to Au⁰, the pre-step for the nucleation of gold clusters.⁴ Graphene provides the nucleation sites for gold clusters, which gradually leads to the epitaxial growth of Au nanobelts. For Au nanowires and Au nanoribbons, graphene template facilitates the coalescence of gold clusters by virtue of “oriented attachment”, which is the unclassical mechanism of paramount importance in the formation of anisotropic structures.

Wednesday, 21/Aug/2019 4:48pm - 5:00pm

Abstract ID: 792 / FBB-2: 5

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biosensors for Imaging

Keywords: Photoacoustic Imaging, Fluorescence, Contrast Agents

A Systematic Approach to Compare Commercial Near-Infrared Dyes for Photoacoustic Imaging

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Photoacoustic Imaging (PAI) is an imaging modality that combines optical and ultrasound imaging. PAI can detect and differentiate between endogenous light absorbing molecules; however, many studies also utilize exogenous contrast agents to locate biological entities or observe biological functions such as lymphatic drainage [1, 2]. Despite the common use of contrast agents for PAI, there are no standard methods to compare and select contrast agents for various applications. Here, we propose a systematic in vitro approach to compare various organic dyes as contrast agents for PAI. A minimum of fourteen concentrations from 0 to 200 μM of the commercially available dyes IRDye800CW, IRDye QC-1, and IRDye CF770 were made in PBS. Triplicate samples were imaged for each concentration and each dye within a light scattering phantom next to PBS as a control using a tomographic PAI device (iThera Medical, Munich, Germany). Analysis was done with the native ViewMSOT software to determine the minimum detectable concentration (MDC) and the quantifiable (or linear) range of concentrations for each dye. The MDC was determined using the EP17 protocols described by Armbruster and Pry [3], and the quantifiable range was determined through statistical methods described in EP6-A [4]. A second experiment was performed to determine the effects of PAI photobleaching (decay in PAI signal) by imaging each dye for one hour using the same experimental set up and analysis software. These two experiments showed that of the dyes tested, QC-1 had the best MDC and was least affected by PA photobleaching; however, it had the smallest quantifiable range. From these observations, QC-1 may be the ideal contrast agent for applications that require repetitive imaging and high sensitivity to the contrast agent; however, IRDye800CW or CF770 may be more desirable when a large range of quantification is required. Furthermore, IRDye 800CW and CF770 are both fluorescent dyes and can also be used for fluorescence imaging validation. In conclusion, no single dye the best contrast agent for all applications of PAI. For each unique application, several PAI contrast agents should be tested to determine which one best meets the requirements.

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Acknowledgments: Canadian Institutes of Health Research, Canada Foundation for Innovation, Henry Farrugia Research Fund and Natural Sciences and Engineering Research Council of Canada CGS-M.

Abstract ID: 793

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Drug delivery/controlled release

Keywords: dasatinib; nanocrystal; antisolvent precipitation; drug release

Dasatinib Nanocrystal and Nanotablets

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Pharmaceutical industry has shown an increasing desire to formulate poorly water soluble drugs as nanoparticulate formulation with the goal of improving dissolution rate, enhancing bioavailability, eliminating food effects, and improving efficacy and safety. Dasatinib, a poorly water soluble drug, is a kind of multitargeted oral tyrosine kinase inhibitors, which is for the treatment of chronic myelogenous leukemia and philadelphia chromosome positive lymphoid leukemia. In this work, dasatinib nanocrystal were prepared via antisolvent precipitation. Various factors that affect particle size and size distribution were investigated. Structure, stability and in vitro dissolution of the as-prepared dasatinib were evaluated. Furthermore, the nanoparticulated dasatinib tablet formula was screened to enhance drug release. The results indicated that dissolution rate of nanotablets was higher than that of raw dasatinib tablet in the both medium of pH 4.5 and pH 6.8, respectively. Therefore, liquid precipitation method would offer a great opportunity for poorly water-soluble drugs to achieve nanoscale particles with a rapid dissolution rate.

Abstract ID: 794

Symposium 2: Functional Composite Materials (FCM)

Invited Talk

Topics: Smart Composites

Keywords: Multiphase microfluidics; Smart Emulsion; Functional Microparticles; Structure control

Droplet-based Microfluidics for Smart Emulsions and Functional Microparticles

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Abstract: Droplet-based microfluidics has recently emerged as a new and promising area of science and technology in the last decades. Preparation of functional materials with microfluidics has attracted great interest from scientist and technologists with different backgrounds and occupations. This work will systematically introduce the recent progress in multiphase flow control in droplet-based microfluidics and preparation of smart emulsions and functional materials with microfluidics mainly by the authors' research group. Controlled multiphase flow with different flow patterns by multiphase microfluidics will be introduced. They have been utilized in novel materials preparation of considerable fields such as optics, biomedicine, controlled porous material and drug release.

Thursday, 22/Aug/2019 3:30pm - 3:42pm

Abstract ID: 795 / FCM-4: 8

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Applications of Composites

Keywords: carbon fiber composite, stress, defect, eddy current, field frequency

Eddy Current on Carbon Fiber Composite

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Carbon fiber composite are widely used. Apart from its high strength/density ratio, carbon fiber composite also has advantage of flexible design ability. Wide applications of the composite range from airplanes to a tennis racket. Carbon fiber is a kind of semiconductor, which has some interesting phenomena when in electromagnetic field.

This paper introduces research on detection of mechanical properties of carbon fiber composite by eddy current technology. The properties include stress, defect and fiber pattern, which are important factors in structure mechanics. With the known properties, the behavior of a structure on duty will be more predictable. On the other hand, an object with such structures is able to show some of its behaviors.

In simulation, we use equivalent eddy current ring theory to describe the induced current in carbon fiber composite. Resistivity tensor is used to characterize electrical property of anisotropic materials. Thus electrical parameters of the eddy current ring is calculated. Equations of the equivalent circuit are obtained from Kirchhoff's law for output of the eddy current sensor.

In experiments, a serious of validation tests were undertaken. These includes effect of composite stress, fiber pattern on eddy current sensitivity; relation between current frequency and its penetrating depth; detect sensitivity to composite defect.

Results of simulation and experiment show that fiber pattern and stress affect the resistance tensor of the composite, while frequency of the eddy current plays a kay factor on field penetration depth. A drilled hole on the composite causes disorder of the eddy current, this offers a way to detect it. Carbon fiber composite with eddy current sensor could be used as smart structures.

Abstract ID: 796

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Concrete and cementitious composites

Keywords: Nanosilica, Metakaolin, Natural Fibers, cementitious composites.

IMPACT OF NANO-METAKAOLIN ON PROPERTIES OF CEMENTITIOUS COMPOSITES

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The process of tailoring of materials using supplementary cementitious materials has been adjudged to help reduced the use of cement which was considered to be a source of carbon dioxide at the point of production and utilization. Hence, this research study the impact of nano-metakaolin, which contain colloid nanosilica and laboratory produced metakaolin, calninated from natural kaolin. The mixture of the nano-metakaolin was used as substitute of binding material up to 12%. The tailoring of these materials with natural fibers produces cementitious composites materials that are more localized and minimal cost. The water cement ratio was targeted at 0.3 with the utilization of superplasticizer. ECC 45 mix design model was adopted and adjusted relative to the aim and objective of the research. The specimens were tested at 7, 28, 56 and 90 days after exposure in ambient temperature and seawater. The result clearly revealed that all specimens with incorporation of nano-metakaolin and natural fibers performed better than the control specimen that does not contain nano-metakaolin and fibers in terms of mechanical properties. The research study also revealed that the binding material can be replaced with nano-silica hence contribute to the reduction of carbon dioxide emission through cement production. In conclusion, this study proffers a better option to binding material and establishes a fundamental basis for further study in terms of binder replacement.

Abstract ID: 797 / Poster: 13

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Thin Film Growth & Epitaxy

Keywords: ϵ -Ga₂O₃; MOCVD; heteroepitaxy; phase transition.

Heteroepitaxy of ϵ -Ga₂O₃ thin films by metal organic chemical vapor deposition

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The research interest in Ga₂O₃ materials is inspired by its ultra-wide bandgap of ~4.9 eV. Baliga's figure of merit for Ga₂O₃ is several times higher than that of GaN and SiC, allowing Ga₂O₃ to be applied in high power and low loss electronic devices [1]. Very recently, theoretical research points out that 2-dimensional electron gas (2DEG) exists in ϵ -Ga₂O₃ due to polarization effect, which contributes to the realization of high mobility ϵ -Ga₂O₃-based devices [2]. However, 1) the growth of ϵ -Ga₂O₃ thin films are always mixed by β -Ga₂O₃ and 2) the crystal quality of ϵ -Ga₂O₃ grown by heterogeneous substrates are low [3, 4]. In this work, Ga₂O₃ thin films were grown by metal organic chemical vapor deposition (MOCVD) using O₂, H₂O, N₂O as oxygen precursors. The temperature range was set to 450~660 °C and the phase transition and phase stability of β - and ϵ -Ga₂O₃ were investigated. It is found that phase pure ϵ -Ga₂O₃ easily forms on c-plane sapphire substrates by using Triethylgallium (TEGa) and H₂O as the precursors. Furthermore, by using two-step growth method, in which the nucleation layer was grown at 600 °C and the epilayer was grown at 640 °C, the crystal quality of ϵ -Ga₂O₃ was effectively improved. The growth mode of ϵ -Ga₂O₃ changed from 3D multi-layer mode to 2D layer-by-layer mode as the temperature raised. We derive high quality ϵ -Ga₂O₃ that is characterized by atomically flat layer-by-layer surface and the screw-type dislocation density determined by X-ray diffraction is as low as $1.8 \times 10^8 \text{ cm}^{-2}$. Nowadays, large-size sapphire is commercially available and cheap. Using sapphire as the substrate for ϵ -Ga₂O₃ could lower the cost of ϵ -Ga₂O₃-based devices and makes them more competitive as next generation power electronics in the semiconductor industry. This work also demonstrates the potential of MOCVD to be used for the heteroepitaxy of high quality ϵ -Ga₂O₃-based materials and devices.

Abstract ID: 798

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Nanomaterials for Biomedical Applications

Keywords: Magnetically Actuated Drug Delivery, Magnetic Nanoparticles, Plasma Polymerization

Composite Magnetic Particles Coated by Plasma Polymerization for Drug Delivery

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The major challenge in the design of drug delivery vehicles (DDV) is the stability of the vehicle. DDV must be stable during administration and circulation until the target site is reached to avoid premature release of the payload. The DDV, however, must be able to release the payload at the target site. To achieve this, DDV that include stimuli-responsive materials have been proposed. The stimuli may be internal, such as changes in pH, or external, such as the application of electromagnetic fields or ultrasound. The use of external stimuli has the advantage of allowing for more control in triggering the drug release. For example, in DDV systems composed of magnetic nanoparticles embedded in thermosensitive polymer particles, drug release can be triggered by an alternating magnetic field (AMF). The AMF induces heat dissipation by the magnetic nanoparticles, which then causes changes in the conformation or degradation of the polymer particle that facilitates the release of the drug. In this contribution, we describe the preparation of a DDV system composed of magnetic nanoparticles embedded in polycaprolactone semicrystalline polymer particles whose melting point can be reached by the heat dissipation induced by AMF. The particles are coated with two materials: A first coating is applied by plasma polymerization. A second external coating with a hydrophilic polymer is chemically attached for stability in aqueous media. Our results show that the plasma polymerization coating is effective in preventing premature drug release, thus resulting in a DDV that is stable before application of the AMF trigger.

Abstract ID: 799

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Applications of Composites

Keywords: Hydrothermal synthesis, Sn²⁺-doped NiO, xylene gas sensor, isovalent doping

Enhanced sensing properties of xylene gas sensors based on Sn²⁺-doped NiO nanostructure

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Xylene with colorless, sweet smelling, and toxic properties is largely emitted by industrial production and building materials, such as oil refining, synthetic fiber, antiseptic materials, and adhesives, etc.[1,2], which can cause headaches, dizziness, irritation of the skin and eyes, and diseases of the memory and nervous systems[3]. Therefore, it is emergent to develop a certain of kind of xylene sensors with high response, relatively low working temperature, and high selectivity. In this work, Sn²⁺-doped NiO microspheres (SNM) with different Sn²⁺ concentrations were synthesized via a facile hydrothermal method and their gas sensing properties to xylene have been investigated. As shown in Figure 1, the results indicate that the way of Sn²⁺ doping for NiO microspheres can significantly enhance the sensing performance to xylene and the SNM with 8% molar ratio of Sn²⁺/Ni²⁺ (SNM-8) has the best response of ~30 to 10 ppm xylene (Response = R_g/R_a, where R_a is the initial resistance in dry air and R_g is the resistance of the sensors in target gases) at the working temperature of 180 °C than other gases. The significant improvement of the response to xylene can be attributed to the change in hole carrier concentration, the adsorbed oxygen species, the crystalline size, and the specific surface area. Additionally, together with other important gas sensing parameters for instance gas response time and operating temperature, the SNM-8 sensor can provide a promising solution in a high response and lower operating temperature with less energy consumption aspects to detect the xylene gas for the real applications.

Key Words: Hydrothermal synthesis, Sn²⁺-doped NiO, xylene gas sensor and isovalent doping

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Abstract ID: 800

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Carbon Nanomaterials

Keywords: graphene derivatives, sensors, dopamine, ascorbic acid, cytotoxicity

Amphiphilic comb polymer modified graphene surfactant for electrochemical sensing of dopamine and ascorbic acid.

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Graphene and its derivatives are widely studied in the development of novel sensors for biological applications. In this work, the evaluation of a new amphiphilic polymer modified graphene surfactant for the sensing of two biologically important molecules, dopamine (DA, a neuro-transmitter) and ascorbic acid (AA, Vitamin C). The amphiphilic modification was achieved by the grafting of pentadecylphenylmethacrylate (PDPMA), derived from a biobased feedstock, to graphene oxide (GO) via atom transfer radical polymerization and subsequently its sulphonation and neutralization. The toxicity studies were performed by MTT assay method and carbon paste electrode (CPE), fabricated using the graphene surfactant, was studied in the electrochemical sensing of dopamine and ascorbic acid (in the concentration range of 0.1mM to 8mM and from 0.5 mM to 7 mM, respectively) in a phosphate buffer solution (0.2 M, pH 7.4). The linear increase of current with the amount of analyte in the buffer solution in, suggesting its suitability for quantitative estimation.

Abstract ID: 801

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Production and characterization of composite materials

Keywords: MOFs composites, in-situ synthesis, adsorption, 2, 4-dichlorophenoxyacetic acid

In-Situ synthesis of UiO-66-NH₂/sponge and highly efficient adsorption 2, 4-dichlorophenoxyacetic acid in water

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In-Situ synthesis of UiO-66-NH₂/sponge and highly efficient adsorption 2, 4-dichlorophenoxyacetic acid in water

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Metal-organic frameworks (MOFs) have been widely used in a variety of applications, including catalysis, separation, and adsorption due to their superior properties, including simple synthesis, high specific surface area, versatility, and chemical/thermal stability. In this work,

UiO-66-NH₂ was used as an adsorbent to remove 2, 4-dichlorophenoxyacetic acid (2, 4-D), one kind of herbicides and preservatives with potential carcinogenicity and mutagenicity, from water. The conditions of adsorption were optimized and the mechanism of adsorption was discussed. Then, UiO-66-NH₂/sponge composites were successfully in-situ synthesized with nitrile rubber sponge as the substrate. The adsorption properties of the UiO-66-NH₂/sponge for removal and enrichment of 2, 4-D in water was studied and compared with UiO-66-NH₂. The prepared composite material showed its advantages in applications with higher absorption effects.

Key Words: MOFs composites, in-situ synthesis, adsorption, 2, 4-dichlorophenoxyacetic acid

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Abstract ID: 802

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: DNA chips and nucleic acid sensors

Keywords: dual signal detection; long noncoding RNA; multiplexed amplification; enzyme-aided target recycling; hybridization chain reaction; electrochemical genosensor.

Double determination of long noncoding RNAs from lung cancer via multi-amplified electrochemical genosensor at sub-femtomole level

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An ultrasensitive electrochemical genosensor has been fabricated for the double determination of two different specific sequences deduced from the maternally expressed gene3 (MEG3) lncRNA (long noncoding RNA), which was demonstrated by coupling RNase A-aided target recycling with DNA supersandwich-induced signal enhancement, based on a composite interface of graphene-like tungsten disulfide/dendritic gold nanostructures (WS2/DGN). Firstly, duple target sequences of T1 and T2 were captured by the primer probes of P1/P2 functionalized Fe₃O₄@C magnetic nanoparticles, via the DNA/RNA hybridization between T1/T2 and P1/P2. In the presence of RNase A, T1 and T2 were released to trigger the target recycling, accompanied by the generation of numerous intermediate DNAs designated as IT1 and IT2, respectively. After the magnetic separation, the IT1 and IT2 were liberated and hybridized with the capture probes of CP1/CP2 loaded DGN/WS2 modified electrode. Subsequently, the stepwise DNA hybridization chain reactions (HCR) labeled with ferrocene (Fc) and methyleneblue (MB) were processed, respectively. The DPV current values of Fc and MB were recorded, which were proportional with the concentration of T1 and T2, respectively. Using the multiple amplification strategy, this newly designed genosensor provided a wide linear range from 1 fM to 100 pM with a low detection limit of 0.25 fM for T1 and 0.3 fM for T2. The application of the genosensor in real serum sample has also been studied, confirming the excellent selectivity and sensitivity for the application in bioanalysis and clinical diagnostics.

Abstract ID: 803**Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)****Oral Presentation***Topics:* Fundamental investigations on low-dimensional nanomaterials and their functional structures properties*Keywords:* Polyenes, Electrochemistry, Spectroscopy, Electronic Properties**Non-Planar Polyenes: a Circuit Boards with Tunable Electronic Properties****Alexey V. Rybalchenko¹, Vera A. Solovyeva¹, Vladimir A. Akhmetov^{1,2}, Natalia S. Lukonina¹, Konstantin Yu. Amsharov², Alexey A. Goryunkov¹**¹Department of Chemistry, Lomonosov Moscow State University, Leninskie Gory, 119991 Moscow, Russi; ²Department of Organic Chemistry, Friedrich Alexander University Erlangen-Nuremberg, Erlangen, Germany; dr.vera.solovyeva@gmail.com

Bowl-shaped polycyclic aromatic hydrocarbons (PAH) or buckybowl are pyramidalized polyenes composed of fused hexagons and pentagons, which can be considered as substructures of fullerenes. Buckybowl demonstrates superior acceptor properties as compared to planar PAH consisted of fused hexagons [1]. Recently reported efficient strategy for the direct synthesis of functional buckybowl [2] significantly broaden scope of synthetically available buckybowl with desired carbon frameworks and side chains [3] which opens a highway to the broad spectrum of derivatives with fine-tuned physicochemical properties with preserved electron accepting properties (due to low disturbance of π -conjugated system), which are essential for fabrication of efficient buckybowl-based organoelectronic devices.

Here we report the features of molecular and electronic structures of indaceno[3,2,1,8,7,6-pqrstuv]picene, indeno[4,3,2,1-cdef:4',3',2',1'-lmno]chrysene, extended indacenopicene and tetraindeno[1,2,3-cd:1',2',3'-fg:1'',2'',3''-jk:1''',2''',3'''-mn]pyren frameworks prepared via fluorine promoted Aryl-Aryl coupling [2,3] as well as related polyaromatic compounds. The derivatives were spectroscopically characterized; their electrochemical behavior, the reduction and oxidation potentials were measured by means of cyclic voltammetry.

The work was supported by Russian Science Foundation (project RSF-18-13-00337)

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Abstract ID: 804

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Lithium Ion Batteries

Keywords: Electrolyte additives, ionic conductivity, solid electrolyte interface

Hydroxy Terminated Poly(dimethylsiloxane) as an Electrolyte Additive to Enhance the Cycle Performance of Lithium-Ion Batteries

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Hydroxy terminated poly(dimethylsiloxane) (PDMS-HT) is used as an electrolyte additive in electrolyte systems containing 1 M LiPF₆ in EC:DMC with solvent ratios 1:9, 3:7, 4:6, and 1:1 v/v to enhance the cycle performance of lithium-ion batteries. In this study, it is observed that adding a small amount of PDMS-HT to the standard LIB electrolyte leads to improved specific capacity as well as improved capacity retention over prolonged cycles. The use of PDMS-HT as an electrolyte additive leads to a slight increase in Li⁺ ion conductivity and has no impact on the electrolyte potential window. Also, the PDMS-HT additive allows the formation of a more stable solid electrolyte interface (SEI) layer that enables the LIB cells to be cycled for longer cycles with minimal capacity fading. This combination of improved ionic conductivity and enhanced SEI layer is due to the PDMS-HT additive provides enhanced electrochemical performance allowing for the cells to surpass standard electrolytes which makes it an excellent candidate for an electrolyte additive for lithium ion batteries.

Abstract ID: 805**Symposium 1: Functional Biomaterials and Biosensors (FBB)****Oral Presentation**

Topics: Additive Manufacturing & bioprinting

Keywords: biofabrication, bioprinting, bioink, thiol-ene cross linking, gelatine

Thiol-ene Clickable Gelatin as Bioink for Biofabrication: Expanding the Fabrication Window through Macromolecular Cross-linkers

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Biofabrication is a young field of research that aims at the automated generation of hierarchical tissue-like structures from cells and materials through Bioprinting or Bioassembly [1]. However, the lack of variety in printable hydrogel systems, which are the mainly used materials for the formulation of bioinks [2], is one major drawback for the advancement of the complete field [3]. Gelatin is often adopted for this purpose, usually modified with (meth-)acryloyl functionalities for post-fabrication curing by free radical photo-polymerization, resulting in a hydrogel that is cross-linked via non-degradable polymer chains of uncontrolled length.

We have introduced GelAGE as a new thiol-ene clickable and broadly applicable alternative for gelatin-based bioinks [4]. The advantage of this system is the absence of non-degradable polymeric components after cross-linking compared to the free radical polymerization, as well as a better control over cross-linking density, and compatibility with Vis-light addressable initiator systems such as (Ru/SPS). Here we present the evolution of this system by stepwise altering the cross-linker from DTT to PEG-dithiol and star shaped 8-armed PEG-octathiol to multi-thiolated hyaluronic acid and finally a Hyaluronan-AGE / thiolated-Hyaluronan bioink as comparison. This led to a continuous improvement of the printability in terms of shape fidelity with decreasing overall polymer concentrations at constant cytocompatibility. We also present biological evaluation of this system for cartilage engineering.

Key Words: Biofabrication, Bioink, Thiol-ene cross linking, biofabrication window

Achnowledgements

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Abstract ID: 806**Symposium 1: Functional Biomaterials and Biosensors (FBB)****Poster Presentation**

Topics: Biomaterials for musculoskeletal regenerative engineering

Keywords: poly(oxazoline), cartilage, tissue adhesive, cartilage integration

Catechol-modified Poly(oxazoline)s with Tunable Degradability Facilitate Cell Invasion and Lateral Cartilage Integration

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Poly(2-alkyl-2-oxazoline)s (POx) are a promising candidate for biomedical applications due to their good cyto- and hemocompatibility. They are also very versatile polymers due to the variety of available functional monomers including vinyl [1] or thiol functionalities [2]. These groups can be used to perform thiol-ene chemistry for further functionalization or to produce hydrogels. We have previously described the introduction of cysteines via thiol-ene chemistry for biopolymer-coupling via native chemical ligation [3].

Here we exploit the thiol-ene coupling to introduce catechol-functionalities as mussel-inspired adhesion moieties for the development of tissue adhesives. Tissue adhesives play an important role in clinical applications and may aid in the treatment of cartilage defects for improved cartilage integration. However, many fail to satisfy the demand for adequate adhesive strength on wet tissue surfaces and to facilitate sufficient cell migration and extracellular matrix (ECM) deposition at the defect site. Utilizing poly(2-alkyl-2-oxazoline) (POx)-based polymers equipped with catechol groups and combining them with the natural wound sealant fibrinogen, we fabricated an adhesive biosynthetic hydrogel with tunable mechanical properties and improved bonding strength. Degradation of the hydrogels could be adjusted by the ratio of amide to ester linkages of the catecholic functional group at the POx side chain. In an in vitro disc/ring model for lateral cartilage integration, a benefit in long-term integration was observed with enhanced degradation of the adhesive without the expense of bonding strength. Incorporation of degradable ester linkages in the polymer facilitated cell invasion and strong deposition of cartilaginous ECM at the defect site. Overall, the results suggest that the presented injectable adhesive hydrogel, due to its easy tunability, holds great potential for cartilage defect treatment and other medical applications.

Key Words: poly(oxazoline), cartilage, tissue adhesive, cartilage integration

Acknowledgements

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Abstract ID: 807**Symposium 1: Functional Biomaterials and Biosensors (FBB)****Oral Presentation**

Topics: Biomaterials for Cardiovascular Applications

Keywords: tissue engineered vascular grafts (TEVGs), melt electrowriting (MEW), biomimetic hierarchical design, vascular smooth muscle cells (vSMCs)

Orchestrating cellular organization and phenotype in small diameter bi-layered vascular grafts by heterotypic scaffold design

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To facilitate true regeneration, a vascular graft should direct the evolution of a neovessel to eventually obtain the architecture and function of a native mature vessel. Hierarchical scaffold design is a crucial parameter to develop appropriate tissue characteristics in the different layers of a vessel. The natural layers of the human vessel, e.g. the tunica intima and the tunica media, can be engineered in bi-layered tubular scaffolds. These scaffolds must permit the adhesion and formation of a confluent endothelial cell monolayer on the intimal side to avoid occlusion via thrombosis. In the medial layer, vascular smooth muscle cell (vSMC) stacking and circumferential alignment must be recapitulated to ensure the contractile function of the vessel. To date, fabrication of an dense luminal fibrous scaffold layer for endothelialization combined with an open fibrous layer for full population by vSMCs with close cell-cell contact throughout the medial layer, remains a challenge in bi-layered scaffolds.

To address these limitations, we present a fabrication approach that combines hierarchically layered scaffold design with the possibility to control structural orientation within the medial layer as guidance for biomimetic vSMC adhesion and growth. This bio-inspired scaffold design was achieved with a novel combination of conventional solution electrospinning and the new melt electrowriting (MEW) technology [1] onto cylindrical targets. The scaffolds consisted of an inner dense randomly oriented layer of single micron diameter fibers, and an oriented outer layer of one order of magnitude thicker fibers and bigger pores. We demonstrate that this vascular graft supported the organization of a continuous luminal endothelial monolayer and multiple oriented layers of vSM-like cells in the outer layer of the graft. Induction of the phenotypic morphology of the endothelium and vSM-like cells was enabled by this specific scaffold hierarchy. This study underlines the importance of the convergence of fabrication techniques to create scaffold designs that can support and control heterotypic cell organization and differentiation, improving vascular tissue engineering strategies.

Key Words: tissue engineered vascular grafts (TEVGs), melt electrowriting (MEW), biomimetic hierarchical design, vascular smooth muscle cells (vSMCs)

Acknowledgements

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Abstract ID: 808 / Poster: 25

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Composites used in automotive industry

Keywords: NAO composites, Fibers, Friction performance

Effects of Several Fibers on the Friction Performance of Non-asbestos Organic Friction Composites

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Several fibers of the non-asbestos organic (NAO) friction composites on the effect of the friction coefficient and the wear rate were investigated. We developed the 1D-2D-3D structure composites of eco-friendly friction materials to replace the NAO friction materials containing copper or some metals or improve the friction performance with a high and stable coefficient of friction, low wear loss, low fade, low noise, and high shear strength. Several fibers such as kevlar, potassium titanate, rock wool, wollastonite, ceramic, glass, copper, steel, etc. and some particulates or laminates materials were employed to form multi-dimensional composites to build the tough structure. The friction composites containing some fibers, binder, lubricants and fillers were finished by mixing using a double cone mixer, pre-compaction, compressive molding, and then heat treatment into a brake pad, which investigated their physical properties, mechanical properties, microstructure, and friction test to study its friction and wear mechanism. This study will build a structure of the robust 1-2-3 dimensions that contain a particular, laminate and irregular fiber configuration, which establishes a concept of having multi-compositions, multi-hardness, multi-size and multi-shape to satisfy a possible braking condition.

Abstract ID: 809

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Plenary**

Topics: Electrochemical Supercapacitors

Keywords: Covalent Organic Framework, Porous Material, Energy Storage

Two-dimensional Covalent Organic Framework for Energy Storage

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Covalent organic frameworks (COFs) are porous materials that are constituted with organic building units and covalent bonds, as a new crystalline porous material, the COFs have been rapidly developed in a short period of several years. In comparison with other crystalline porous solids (Inorganic zeolites and hybrid MOFs), the COF materials possess the advantages of high surface areas and stable porosity, and porous channels are arranged in order with an adjustable internal environment. It is precisely because these advantages are combined with conventional pore structures that COF materials can show numerous potential applications in different fields of research. The 2D-COF porous structures with ultrahigh surface areas and intrinsic heteroatom doping are extremely favorable for enhancing the electrochemical performances. Their controllable structures also make it possible to deeply study the mechanism and structure-performance relationships in electrochemistry. Therefore, the 2D-COF materials have a wide application prospect in energy storage.

Abstract ID: 811

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalysis and Energy

Keywords: Keys: Molecular dynamics, [Al]₈ [Cu]₄ [Fe]₁, [Al]₂₇ [Cu]₁₀ [Fe]₅ and [Al]₃₄ [Cu]₁₄ [Fe]₇ clusters

Molecular Dynamic Studies on the evolution of [Al]₈ [Cu]₄ [Fe]₁, [Al]₂₇ [Cu]₁₀ [Fe]₅ and [Al]₃₄ [Cu]₁₄ [Fe]₇ Icosahedral Quasicrystal using DFT

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Computer simulation methods, such as Monte Carlo or Molecular Dynamics, are very powerful computational techniques that provide detailed and essentially exact information on classical many-body problems. Evolution of Icosahedral quasicrystal [Al]₈ [Cu]₄ [Fe]₁, [Al]₂₇ [Cu]₁₀ [Fe]₅ and [Al]₃₄ [Cu]₁₄ [Fe]₇ clusters were presented. It was observed the fluctuations of total energies and conserved Hamiltonian was due to potential energy and kinetic energy respectively. Also stability behavior due to the instantaneous temperature makes the thermostat efficient. However, Ir-spectrum extracted from the trajectories of the fourier transform of the dipole-dipole auto-correlations are presented and are in agreement with Mansur and Babaji, 2016 & Rudenko and Mazurenko 2007.

Abstract ID: 812

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Drug delivery/controlled release

Keywords: resveratrol, nanoliposomes, high pressure microfluidization, anti-tumor

Novel nanoliposomes for resveratrol through high pressure microfluidization: characterization and stability evaluation

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Resveratrol (RSV) nanoliposomes prepared by high pressure microfluidization (HPM) were investigated based on the encapsulation efficiency, transmission electron microscopy (TEM), size distribution and zeta potential. In addition, the stability of resveratrol nanoliposomes was evaluated at different pH, temperature, and storage conditions. Results showed that with the increasing of pressure (from 10000 to 18000 PSI) and cycle (from 1 to 3) of microfluidization, the particle size decreased and the encapsulation efficiency increased. The nanoliposomes obtained at conditions of 18000 PSI and 3 cycles had a considerably high encapsulation efficiency (87.74±1.01%) and zeta potential (-55.5 mV). Dynamic light scattering (DLS) indicated that the particle size was below 100 nm, which was confirmed by TEM analysis. The nanoliposomes showed better stability at alkalescence and low temperature. Furthermore, the RSV nanoliposomes was stabilized at 4 °C for 50 days with the retention percentage above 95 %. Dynamic dialysis experiment showed that resveratrol nanoliposomes released for 26 h, 13 times of free resveratrol, which indicated significant delayed releasing effect. The cell experiments in vitro demonstrated that the inhibition ratio of resveratrol nanoliposomes to hepatoma carcinoma cell HepG2 and gastric carcinoma cell AGS were 77.36% and 72.64% respectively, higher than resveratrol group and resveratrol with blank nanoliposomes group, indicating a good antitumor effect.

Abstract ID: 813

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Electrochemical Supercapacitors

Keywords: 2D nanomaterials, Energy Storage, Electrochemical capacitor

Ultracapacitive Energy Storage Using 2D Nanomaterials Under Extreme Conditions

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With increasing demand for high performance energy storage devices, the feasibility of reliable and functional energy storage devices that well operates under extreme conditions is of prime importance for expanding applicative fields as well as for understanding materials' intrinsic and extrinsic properties and device physics. In this talk, I will introduce the control in the physical structure and chemical composition of 2D nanomaterials for ultracapacitive energy storage devices under limited circumstances, where conditions are classified into thermodynamic (e.g. pressure, volume and temperature) and kinetic (e.g. high rate and frequency) variables.^{1,2} In addition, a fundamental foundation via in-situ spectroscopic techniques will be presented to understand charge storage phenomenon of new materials and devices occurring on a nanoscale under various circumstances.¹

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Abstract ID: 814

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Mechanical and physical properties

Keywords: Finite element method, Gadolinium, Duplex stainless steel

FEM Analysis on the Cold Rolled Gd-B-Duplex Stainless Steels

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Finite element method (FEM) analysis is required to find an optimum cold rolling condition of the Gd-B-duplex stainless steels for the storage and transportation of the spent nuclear fuel (SNF) because the process may introduce surface cracks of the alloy. The objective of this study is to find an optimum condition of cold-rolling process of the Gd-B-DSTS by FEM. FEM analysis to find an optimum cold rolling condition was carried out by modelling based on the cold roller size and materials values of the Gd-B-duplex stainless steels. The duplex stainless steels to confirm FEM analysis were prepared by inductive melting and casting followed by hot rolling. The hot rolled specimens with 5 mm thick were cold rolled to be 1 and 3 mm thick, separately. The mechanical properties of the stainless steels were determined by universal testing machine (RB302ML, R&B, Korea). The morphology of the deformed surface of the specimen was observed by optical microscopy. The ultimate tensile strength, yield strength and elongation of the cold rolled Gd-B-stainless steels were measured. The cold-rolling with 25% of reduction of area (RA) of the Gd-B- duplex stainless steels showed that the strain of the left side, right side and center area of the specimen were 35%, 36% and 54%, respectively. For 15% of RA, the strain decreased about 19%, 18% and 34%, respectively. In case of 10% of RA, the strain of the left side, right side and center area of the specimen were 11%, 12% and 17%, respectively. This means that less than 10% of RA is one of the cold rolling conditions not to form surface cracks because of the lower value than the elongation. Visual and optical inspections of the cold rolled specimen also supported the FEM analysis result.

Abstract ID: 815

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Composite structural materials

Keywords: Copper–zinc–iron multinary spinel, hierarchical microstructures, solar light harvestings, physicochemical properties, structure activity relationship

Relationships Between Crystal, Internal Microstructures, and Physicochemical Properties of Copper–Zinc–Iron Multinary Spinel Hierarchical Nano-microspheres

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Rational design and fabrication of high quality complex multicomponent spinel ferrite with specific microstructures and solar light harvestings toward CO₂ reduction and antibiotic degradation to future energetic and catalytic applications are highly desirable. In this study, novel copper–zinc–iron multinary spinel hierarchical nano-microspheres (MSHMs) with different internal structures (solid nano-microspheres, yolk–shell hollow nano-microspheres, and double-shelled hollow nano-microspheres) have been successfully developed by a facile self-templated solvothermal strategy. The morphology and structure, optical, as well as photoinduced redox reactions including interfacial charge carrier behaviors and the intrinsic relationship of structure–property between intrinsic nano-microstructures and physicochemical performance of copper–zinc–iron ferrite MSHMs composites were systematically investigated with the assistance of various on- and/or off- line physical–chemical means and deeply elucidated in terms of the research outcomes. It is demonstrated that the modification of the interior microstructures can be applied to tune the catalytic properties of multinary spinel by tailoring the temperature programming to fine control the two opposite forces of contraction (Fc) and adhesion (Fa). Among various internal microstructures, the obtained double-shelled copper–zinc–iron MSHMs exhibited the superior catalytic performance toward 8.8 and 38 μmol for H₂ and CO productions as well as 80.4% removal of sulfamethoxazole antibiotics. As evidenced from primary characterizations, for example, combined steady-state PL, ns-TAS, and Mössbauer and sequential investigations, the remarkable improvements in the catalytic activity can be primarily attributed to several crucial factors, for example, the more effective e⁻-h⁺ spatial separations and interfacial transfers, multiple internal light scattering, higher photonic energy harvesting and effective reactive oxygen species generation with long radical lifetimes. The current research provides new insights into the molecular design of novel copper–zinc–iron multinary spinels and the intrinsic relationship of structure–property between interior structures (e.g., different crystal texture, morphologies structures) and the physicochemical performance of the aforementioned multinary spinels.

Abstract ID: 816

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Multifunctional composites

Keywords: Ni substituted Bismuth Ferrite, microwave device

Ni substituted bismuth ferrites; Design and testing of broad-band Microwave Monolithic Filter and phase shifter

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Recently, low-power multiferroic based microwave components have potential to lower the size, weight, and power needs of future generation of communication systems¹⁻². Multiferroic materials consists of both magnetic and ferroelectric phase and they offer the possibility of magneto-electric coupling. The purpose of this research is to show wide-band application of multiferroics (BiFe_{1-x}Ni_xO₃) nanoparticles (NPs). The NPs showed magnetic field control of the ferromagnetic resonance (FMR) frequency. NPs of BiFe_{1-x}Ni_xO₃ (x=0.01 -0.1) were prepared by sol-gel method. The XRD study confirms the formation of pure phase bismuth ferrite. Average particle sizes as found from the TEM images were ~ 80 nm. Magnetic hysteresis study confirms ferromagnetism enhancement of Ni-BFO over BFO (10-folds).

Monolithic microwave² band-stop filters and phase shifters were designed and fabricated in coplanar waveguide (CPW) geometry. BiFe_{1-x}Ni_xO nanoparticles were deposited using electrophoretic deposition method on CPW. Filter and phase shifter response were recorded at frequency-sweep mode. As seen above the operating frequency was tuned by application of magnetic field (H) over a wide range (5 to 25 GHz) with a field up to 15 kOe. This results in a tunability of 1.4 GHz/kOe. The pass-band insertion loss is ~3dB and return Loss is >-12 dB. The stop-band suppression is > -10 dB. Addition of Ni into BFO tuned the center frequency from 18 to 21.5 GHz (Fig.C) and band-width of 3 GHz(Fig.D). This is in agreement with the VSM data Fig. (C) and (D). The operating frequency can also be tuned by voltage (V).

The designed phase shifter can be controlled with magnetic field from 0 to 15 kOe. This provides a continuously variable phase shift of 10 to 120 degrees at 25 GHz (Fig.C), with consistent low insertion loss versus phase shift and frequency. A typical low phase error of ±15 degrees over a wide bandwidth is observed.

In order to produce same phase shift, conventional phase shifters require much-increased RF device size than the proto-type BiFe_{1-x}Ni_xO₃ NPs-based phase shifters. The designed phase shifters can be used for electronic steering of antenna arrays and for 5G applications.

Abstract ID: 817 / Poster: 21

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Thin Film Growth & Epitaxy

Keywords: composite films, Ar/O₂ ratio, CaZrO₃, surface morphology, crystal structure, RF sputtering

The effects of Ar/O₂ ratio on the structure and properties of CaZrO₃/Ca_{0.15}Zr_{0.85}O_{1.85} composite films

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The CaZrO₃/Ca_{0.15}Zr_{0.85}O_{1.85} composite films have been prepared using the by the radio-frequency (RF) magnetron sputtering under the different ratios of Ar/O₂. We have studied the effects of the different gas concentrations (Ar/O₂) on a crystal structure, a surface morphology, and electrical properties of the CaZrO₃/Ca_{0.15}Zr_{0.85}O_{1.85} composite films. The surface and the structure investigations have shown a strong influence of the growth conditions on the film microstructure. Both the structural analysis and surface morphology revealed that all grown films are polycrystalline and two-phase. It was found that increasing Ar/O₂ ratio results in an improvement of the structural quality of the CaZrO₃ films and the reduction of Ca_{0.15}Zr_{0.85}O_{1.85} phase. Further, increasing Ar/O₂ ratio results in an increase in surface roughness and grain size for the as-deposited samples.

Thursday, 22/Aug/2019 2:12pm - 2:24pm

Abstract ID: 818 / FESC-2: 2

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

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

Keywords: Molecular dynamics, nanoresonators, damping, dissipation

Atomistic Simulations of Energy Dissipation in Amorphous Silica Nanoresonators

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Nanomechanical resonators are promising as they are ultrasensitive and can be used as sensors, energy harvesters. However, as demonstrated by latest experiments, the capabilities of these devices squarely depend on their mechanical quality factors, Q , defined as the ratio of the stored mechanical energy in the structure to the energy dissipated per period of oscillation. Studying various sources of damping in nanoresonators using experimental techniques is difficult as many of these mechanisms cause dissipation simultaneously. Classical molecular dynamics (MD) simulations were previously used for predicting energy dissipation in nanoresonators and were compared with various theoretical models [1, 2]. However, the accuracy of such predictions of Q and the contributions from different underlying mechanisms squarely depend on the accuracy of the interatomic potential (IP). As the IP parameters are fitted to limited dataset, transferability problems can arise with the possibility of inaccurate predictions. Furthermore, a direct comparison of Q from MD simulations for various materials to experimental data is difficult due to the lack of availability of experimental data. To this end, I would discuss results from MD simulation of damping in amorphous silica as a test case due to the availability of an exhaustive set of measurements of Q for this material. Various interatomic potentials will be used to predict damping in amorphous silica as functions of temperature and frequency. The predictions of Q using published IPs will be compared with experimental measurements. Finally, the mechanisms of dissipation will be discussed.

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Thursday, 22/Aug/2019 9:18am - 9:30am

Abstract ID: 819 / FCM-2: 7

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: Carbon nanotube yarn, stretching, twisting, tetrabromaurate (KAuBr₄)

Highly conductive carbon nanotube yarns with improved strength

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Due to their outstanding mechanical, electrical and thermal properties, carbon nanotubes (CNTs) have been investigated for developing high-performance engineering macrostructures [1,2]. However, macroscopic assemblies made up of carbon nanotubes (CNTs) exhibit properties significantly far below theoretical predictions due to weak load transfer and interfacial interaction between bundles. In the present work, an efficient method for processing highly conductive and high strength carbon nanotube yarns has been developed. First, commercially available CNT yarn materials are aligned by stretching and densified by wet twisting. Then, they are chemically doped in aqueous solutions of potassium tetrabromaurate (KAuBr₄). Microstructures of prepared materials are characterized by electron microscopies and their mechanical properties and electrical conductivity are measured accordingly. After consolidation and doping, the CNT yarn drastically increases the tensile strength, Young's modulus, and electrical conductivity from 60±10.0 MPa, 0.7±0.2 GPa, and 1.0x10⁵±0. 2x10⁴ S/m (pristine) to 1.2±0.1 GPa, 49.3±5.2 GPa, and 1.8x10⁶±7x10⁴ S/m (post processed), respectively.

The stretching, densification and doping process leads to aligned CNTs, closer packed CNTs, and a reduced charge transfer barrier, resulting in enhanced mechanical properties and electrical conductivity [3,4].

Abstract ID: 820

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Magnetic Nanomaterials for Applications

Keywords: Perovskite-based Manganites, ferromagnetic resonance, relaxation mechanism

Magnetization dynamics in La_{1-x}Sr_xMnO₃ nanoparticles

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Perovskite-based Manganites have been the subjects of intense research because of their potential use as microwave tunable devices. They exhibit a variety of transport and magnetic properties that sensitively depend on the stoichiometry and structure of the materials [1]. La_{1-x}Sr_xMnO₃ is a intensively used composition due to its excellent magnetic properties. At low doping level La_{1-x}Sr_xMnO₃ consists only Mn³⁺ ion hence it shows low magnetism at room temperature. By increasing doping of divalent Sr ions due to strong Hund's coupling Mn³⁺ starts conversing to Mn⁴⁺ proportional to doping percentage and increment of Mn⁴⁺ ions derives double exchange that mediates ferromagnetism in La_{1-x}Sr_xMnO₃ [1,2].

We have synthesized La_{1-x}Sr_xMnO₃ (with x=0.1,0.3,0.5) nanoparticles(NPs) using one-step sol-gel citrate method and calcined at 1000° C. XRD pattern confirm the phase formation and highly intense peaks show polycrystalline nature of NPs. At lower doping level the phase of La_{1-x}Sr_xMnO₃ is rhombohedral and at higher doping it is cubic[3]. The average crystalline size calculated from XRD is 30nm. The VSM curve shows (Fig.a) the effect of Sr doping in La_{1-x}Sr_xMnO₃ NPs. On increasing the Sr doping the Magnetization (Ms) & coercivity (Hc) both increases till x0.3, but at x=0.5 Magnetization (Ms) & coercivity (Hc) decreases. Sr doping x = 0.3 has the most appropriate Mn⁴⁺ ion content (Mn⁴⁺/Mn³⁺≈1) for the double exchange interaction (Mn⁴⁺–O– Mn³⁺) while the other samples have more pairs of ions Mn³⁺–O– Mn³⁺ (x<0.3) or Mn⁴⁺–O– Mn⁴⁺ (x>0.3), which result in less double exchange interactions and thus a reduction in Ms[4] thereafter.

We have performed ferromagnetic resonance (FMR) studies extensively from 4 to 21 GHz for all samples (Fig.b). Fig. (c) shows resonance fields (Hr) vs. frequency for all three composition. Hr increases as frequency increases. Value of Hr is largest for x=0.3 at any particular frequency, this is in agreement with VSM data. In Fig. (d). shows line width vs. frequency for different composition.

To verify the relaxation mechanism in LSMO NPs we have considered both intrinsic and extrinsic damping torques. The FMR linewidths are fitted with a micromagnetic model consisting of intrinsic (α) and (β) damping parameters. Hence both the intrinsic and extrinsic damping contributions to linewidth are taken care of. From the experimentally observed resonance fields and linewidths data, we have calculated Gilbert damping factor, intrinsic and extrinsic line width, Gyromagnetic ratio (γ) by fitting the data.

Thursday, 22/Aug/2019 3:51pm - 4:03pm

Abstract ID: 821 / FESC-2: 10

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Nanostructured materials for advanced batteries

Keywords: Keywords: PVDF HFP, Zirconium oxide (ZrO₂) NPs, piezoelectricity and piezoelectric nanogenerator.

Use of ZrO₂ Stimulated PVDF HFP Composite Flexible Thin Film in developing High Performance Piezoelectric Nanogenerator and Transparent Single Electrode Triboelectric Nanogenerator

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ABSTRACT

Piezoelectric nanogenerators (PENGs) have been emerged as one of the most promising approaches for harvesting electrical energy from mechanical and bio-mechanical energy for low power electronic devices. Here we report our studies on transparent, light weighted, flexible, long lasting, environment-friendly and cost effective piezoelectric nanogenerator (PENG) with excellent output characteristic. High open circuit output voltage and power density using flexible Zirconium oxide (ZrO₂) manipulated electroactive poly vinylidene fluoride–hexafluoropropylene (PVDF HFP) nanocomposite films, have been observed. In ZrO₂/PVDF HFP, ZrO₂ act as the catalytic agents for electroactive polymorph nucleation and enhancement of dielectric properties. Compared to previously reported PVDF HFP assisted prototype nanogenerators, this recently developed PENGs exhibits excellent piezoelectric energy harvesting performance with very high power density, high energy conversion efficiency and highly durable. The developed piezoelectric nanogenerator exhibit a large value of open circuit voltage (V_{oc}~120 Volt) and short circuit current (I_{sc} ~1.95 μA) under periodic finger imparting with high power density ~ 7091μWcm⁻³. Fabricated flexible piezoelectric nanogenerator is capable to instantaneous light up commercially available 55 number of blue LED connected in parallel connection. High capacitor charging performance is also observed such as 2.2 μF capacitor has been charged up to 3.5 V just a 17 second time interval. Moreover, Single electrode based triboelectric nanogenerator, fabricated by same composite film, has shown remarkable output voltage (~ 7V) by figure touch.

Wednesday, 21/Aug/2019 6:12pm - 6:27pm

Abstract ID: 822 / FBB-2: 12

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Invited Talk

Topics: Antimicrobials

Keywords: Cu-Ag NP, *Shigella flexneri*, Shigellosis, multi-drug resistance, Balb/c mice, cell toxicity.

Synthesis, Characterization and Anti-Shigellosis Potency of Cu-Ag Bimetallic Nanoparticle

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Human diarrheal diseases caused by different entero-toxicogenic bacteria represent a major health problem in developing countries. From diarrheal patients, the most frequently isolated bacterial pathogen is reported to be the bacterial genus *Shigella*. Generation of resistance to antibiotics is gradually growing among *Shigella* with rising incidence of shigellosis and thus increasing human populations in *Shigella* species-endemic areas. This obsolescence of antibiotics has made it imperative to research on the development of new drugs against diarrheal diseases. In this regard, different metallic nanoparticles (NPs) viz., silver, copper etc. are reported to have potential anti-bacterial action. Therefore, we venture to synthesize copper-silver (Cu-Ag) bimetallic NP, with a view that the particle of dual metals may be more effective as antibacterial drug than that of the individual ones. Here we report about a robust method of synthesis of Cu-Ag NP, its physico-chemical characteristics and anti-shigellosis efficacy *in vitro* and *in vivo*.

In our method, Cu-Ag bimetallic NP has been synthesized by a method of successive reduction of $\text{Cu}(\text{NO}_3)_2$ and AgNO_3 , using hydrazine hydrate as the reducing agent and gelatin and polyvinyl pyrrolidone (PVP) as the capping agents. The particles are core-shell in structure with Cu⁰ core and Ag⁰ shell, about (100 ± 10) nm in size and kill deadly diarrhea-causing multidrug-resistant bacterium *Shigella flexneri* 2a (IDH.4267, tetR, ampR, cipR, nalR, strR, eryR, norR, ofxR, sxtR, chlR), both in test tube and in infected mice. The minimum inhibitory concentration (MIC, 4.0 $\mu\text{g/ml}$) and minimum bacteriocidal concentration (MBC, 5.13 $\mu\text{g/ml}$) of the NP for *S. flexneri* 2a are quite low than the corresponding doses of any antibiotic used. When the shigellosis is induced in Balb/c mice by intra-peritoneal injection of *S. flexneri* 2a, the occurrence of a) mushy stool excretion, b) colon length shortening, c) weight loss and d) bacterial colonization in gastrointestinal tract of mice is significantly reduced by treatment with Cu-Ag NP through oral administration, at a dose of 0.2 mg/gm body weight. The infected mice with gradual weight loss and weakness die within 7 days of infection, whereas subsequent treatment of infected mice with Cu-Ag NP keeps them alive with normal behavior, even up to 30 days. Moreover, the cytotoxicity of the NP is quite low; when checked over normal liver (WRL68) and lung (WI38) cell lines *in vitro*, the MBC dose of the NP killed only about 22.5% of the cells [1].

The prepared Cu-Ag NP, by our simple economic method, can therefore be developed as a potential drug against shigellosis-like diarrheal diseases, which may be highly useful to developing countries with limited health care budgets.

Key Words: Cu-Ag NP, *Shigella flexneri*, Shigellosis, multi-drug resistance, Balb/c mice, cell toxicity.

References

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Thursday, 22/Aug/2019 2:36pm - 2:48pm

Abstract ID: 823 / FESC-2: 4

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Nanogenerators and self-powered nanosystems

Keywords: Piezoelectric nanogenerator, PVDF/CuS NRs, Dielectric constant

Fabrication of flexible thin film Piezoelectric Nanogenerator and Single Electrode Triboelectric Nanogenerator for Energy Harvesting by using CuS nanoparticle doped PVDF

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Recently, polyvinylidene fluoride (PVDF) and its copolymer-based nanocomposites possessing high dielectric constants, have drawn great attention as a suitable candidate for next generation energy harvesters such as piezoelectric nanogenerators, energy storage devices, photovoltaic self-charging cells etc. In the present study, we demonstrate a simple and high performance flexible piezoelectric nanogenerator (PENG) using CuS nanoroses (NRs) doped electroactive PVDF thin film. About 82% electroactive β phase nucleation is achieved by incorporating 5 mass% CuS nanoparticles in PVDF matrix. The interface between the polymer milieu and the NRs leads the critical role in the confinement of the more piezoelectric β phase, resulting in the radical increase in dielectric constant (~ 40.6) of modified NRs composite thin film as compared to pure PVDF thin film. This functionalized PVDF/CuS NRs composite thin film is used to devise a piezoelectric nanogenerator for generating electrical energy from the mechanical energy which is abundantly available in living systems. Maximum open circuit voltages produced in this nanogenerator by normal human finger pressure is ~ 83 V, which is capable of instant lightening of 35 blue LEDs connected in series. The composite thin film has been subsequently employed in Single electrode based triboelectric nanogenerator and significant output voltage (~ 6 V) has been produced by mere figure touch.

Keywords: Piezoelectric nanogenerator, PVDF/CuS NRs, Dielectric constant

Abstract ID: 824

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Electrochemical Supercapacitors

Keywords: hydrophilic carbon cloth; CV, EIS, Electrode material

Chemically Activated Hydrophilic Carbon Cloth as an Electrode Material for Energy Storage Device

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In this work, hydrophobic carbon cloth (HCC) was chemically activated by facile oxidation method using a mixture of concentrated acid consisting of H₂SO₄:HNO₃ (3:1 v/v) followed by NH₄OH treatment. It was found that the treated carbon cloth (TCC) turned hydrophilic on this treatment showing a decrease in contact angle from 145.15° to 72.95°. Fourier-transform infrared spectroscopy (FTIR) confirmed that the oxidation process generates -C=O and CO-NH groups on the surface of TCC which was the indication of the removal of loosely bonded carbon fibers and formation of fine porous carbon structures. Moreover, the surface area of the TCC was increased by 18 times to that of HCC confirmed by Brunauer–Emmett–Teller (BET) analysis. Field Emission Gun Scanning Electron Microscopy (FEGSEM) images showed deeper grooves on the surface of TCC which exhibit surface roughness. On performing a scanning probe microscope (SPM) analysis, the roughness value was found to be 28.9 nm. The electrochemical properties of TCC was investigated using cyclic voltammetry (CV), constant current charge discharge (CCCD) and electrochemical impedance spectroscopy (EIS). The specific capacitance of the TCC measured by CCD was 908.63 mF cm⁻² at 1.5 mA cm⁻² in 1 M H₂SO₄ aqueous electrolyte. Furthermore, CV and EIS studies also depicted a significant increase in the current range and a drastic reduction in resistive behaviour of TCC. These results revealed that the TCC as an electrode material provides good electrochemical performance for energy storage device applications.

Abstract ID: 825

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Nano and Environmental catalysis

Keywords: Selenium catalyst, Nanoparticles, Antioxidant, Free radical

Aqueous Selenium Nanoparticles (ASeNPs) as Antioxidant catalyst

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Aqueous Selenium Nanoparticles (ASeNPs) was synthesized by using sodium selenite as precursor and Gallic acid (GA) as reducing agent. The structure, size, morphology and antioxidant activity of ASeNPs were characterized by High resolution transmission electron microscopy (HRTEM), Ultraviolet-Visible Spectroscopy (UV-vis), Dynamic Light Scattering (DLS), Energy dispersive X-ray spectroscopy (EDAX), Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-AES) and Fourier transform infrared (FTIR). The catalytic activity of the prepared ASeNPs tested as antioxidant for 1, 1-diphenyl-2-picrylhydrazyl (DPPH). Synthesized ASeNPs showed uniform sphere-shaped with average particle size range of 98 nm (HRTEM). EDAX analysis confirmed the presence of selenium in nanosphere. The concentration of selenium nanoparticles in ASeNPs was estimated by using ICP-AES analysis at pH 6, 6.5, 7 and 7 buffer solutions as 210.9, 269.1, 172.9 and 207.6 ppm respectively. FT-IR analysis confirmed the presence of carboxyl (-C=O), hydroxyl (-OH), alkyl (C-H) functional groups at the surface of ASeNPs. ASeNPs exhibited excellent antioxidant activity against DPPH through their hydrogen/electron transfer ability. This study suggested that the ASeNPs were responsible for the replacement of free radical available at nitrogen atom present in DPPH and converted it to 1, 1-diphenyl-2-picrylhydrazine (DPPH-H). The Scavenging of DPPH (%) of ASeNPs followed the sequence of pH 7 buffer > pH 6 > pH 7 > pH 6.5 (Figure 1(a)). The DPPH radical scavenging activity of ASeNPs without any stabilizer or capping agent in this work reached higher than 80% at the concentration of 0.4 mM. Apparent rate constant (kapp) for free radical scavenging reactions of DPPH also calculated and it increases linearly with increase in concentration of ASeNPs. The increase in the kapp value was because of the accessibility of more interaction sites of ASeNPs.

Abstract ID: 826

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Advances in Enzymatic and Non-Enzymatic Biosensors

Keywords: tissue plasminogen, streptokinase, magnetic nanoparticles

Delivery of tissue plasminogen activator and streptokinase magnetic nanoparticles to target vascular diseases

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Thrombolytic therapy for acute myocardial infarction standardly makes use of the medications streptokinase (SK) and tissue plasminogen activator (tPA). In this study, the potential of silica-coated magnetic nanoparticles (SiO₂-MNPs) as nanocarriers clinical thrombolytic therapy was investigated. SiO₂-MNPs for use in targeted therapeutic delivery of tPA and SK were prepared using a combined technique incorporating controlled precipitation and hydrothermal methods. Response surface methodology (RSM) was employed to evaluate the efficiency of the SiO₂-MNPs. The production of SK secreted from *Streptococcus equi* was enhanced using random mutagenesis. The tPA and SK A were encapsulated by means of a silanizing agent with a surface rich in 3-aminopropyltrimethoxysilane layered around the SiO₂-MNPs. Blood clot lysis assays and fibrin-containing agarose plates were used to carry out in vitro thrombolysis testing. The optimum conditions for producing MNPs were found to be at pH = 13 and at a temperature of 75 °C for 45 min. Culture conditions of 2.75% NaCl concentration at initial pH = 7.5 for 90 s under UV resulted in maximum SK activity. The tPA/SK-conjugated SiO₂-MNPs (SiO₂-MNP-tPA-SK) increased operating stability in whole blood and storage stability in a buffer by 92%. More effective thrombolysis using magnetic targeting was indicated by a 38% reduction in blood clot lysis time achieved with SiO₂-MNP-tPA-SK compared to administering the SiO₂-MNPs without guidance. The silica-coated magnetic nanocarriers developed in this study show potential for improved clinical thrombolytic therapy.

Abstract ID: 827

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Invited Talk

Topics: Nanogenerators and self-powered nanosystems

Keywords: Tribotronics, Triboelectric potential, Active mechanosensation, Power management, Self-powered systems

Tribotronics for Mechanosensation and Self-Powered Microsystems

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Tribotronics has attracted great attentions as a new research field about the control and tuning of semiconductor transport by triboelectricity. Here, the tribotronics is firstly reviewed for active mechanosensation and human-machine interfacing. As the fundamental component, contact electrification field-effect transistor is analyzed, in which the triboelectric potential could be used to control the electrical transport in semiconductors. On the basis, several tribotronic functional devices have been developed including tribotronic smart skin, tactile sensing array and tuning diode, which has demonstrated triboelectricity-controlled electronics and established the active mechanosensation for external environment. In addition, the triboelectric power management strategy is also reviewed, in which the triboelectricity can be managed by electronics in reverse action. With the implantation of triboelectric power management module, the harvested triboelectricity by various kinds of human kinetic and environmental mechanical energy could be effectively managed as a power source for self-powered systems. By the research prospects for interactions between triboelectricity and semiconductor, tribotronics is expected for significant impacts and potential applications in MEMS/NEMS, flexible electronics, robotics, wireless sensor network, and Internet of Things.

Abstract ID: 828

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Biomaterials for hard tissue applications

Keywords: Temporal bone; Mesenchymal stromal cells; Scaffold; Osteogenesis; Ear function; Cholesteatoma

The transplantation of hBM-MSCs increases bone neo-formation and preserves hearing function in the treatment of temporal bone defects.

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Temporal bone reconstruction is a persisting problem following middle ear cholesteatoma surgery. Seeking to advance the clinical transfer of stem cell therapy we attempted the reconstruction of temporal bone using a composite bioartificial graft based on a hydroxyapatite bone scaffold (CEM-OSTETIC®) combined with human bone marrow-derived mesenchymal stromal cells (hBM-MSCs). The aim of this study was to evaluate the effect of the combined biomaterial on the healing of postoperative temporal bone defects and the preservation of physiological hearing functions in a guinea pig model. The treatment's effect could be observed at 1 and 2 months after implantation of the biomaterial, as opposed to the control group. The clinical evaluation of our results included animal survival, clinical signs of an inflammatory response, and exploration of the tympanic bulla. Osteogenesis, angiogenesis, and inflammation were evaluated by histopathological analyses, whereas hBM-MSCs survival was evaluated by immunofluorescence assays. Hearing capacity was evaluated by objective audiometric methods, i.e. auditory brainstem responses and otoacoustic emission. Our study shows that hBM-MSCs, in combination with hydroxyapatite scaffolds, improves the repair of bone defects providing a safe and effective alternative in their treatment following middle ear surgery due to cholesteatoma.

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Abstract ID: 829

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Biocomposites

Keywords: Bio-cellulose, composites, Bone tissue regeneration

Bio-cellulose-chitosan based biomimetic composites for potential application in bone tissue regeneration

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Bio-cellulose (BC) produced by certain microbial species represent the purest form of cellulose having much superior physical, mechanical and biological properties than plant cellulose. Being blessed with 3D network structure BC has been reported as an ideal material for composites synthesis for multiple applications. Its composites with nanomaterials, polymers, clays, proteins and so many materials have been reported for biomedical, conducting, electric and relevant applications. Herein, we utilized porous 3D BC framework as scaffold for incorporation of chitosan (Ch) and synthesizing BC-Ch composites. The BC-Ch composite was then utilized as template for in-situ hydroxyapatite (Hap) formation and surface deposition. The synthesized biomimetic composites exhibited high tensile properties and biocompatibility. Morphological analysis made through FE-SEM indicated the porous geometry of bare BC that was covered by chitosan layer in BC-Ch composites and contained homogenously distributed spherical HAp particles in BC-Ch-HAp composites. The synthesized composites showed excellent cell growth and proliferation capabilities against osteoblast cells augmenting their potential application for bone tissue regeneration.

Wednesday, 21/Aug/2019 4:00pm - 4:15pm

Abstract ID: 830 / FC: 1

Symposium 3: Functional Catalysis (FC)

Invited Talk

Topics: Catalysis and Energy

Keywords: Nano-electrocatalysts, Nanoparticles, Rhodium, Platinum, graphene

Replacing Platinum with a Better Performance For HER by the Metal of Wilkinson's Choice

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Proton exchange membrane fuel cells (PEMFC) were used in the NASA Gemini series of spacecraft. Current research on catalysts for PEMFC is based on obtaining higher catalytic activity than the standard carbon-supported platinum particle catalysts. In search of a more sustainable catalyst other than platinum for the catalytic conversion of water to hydrogen gas, a series of transition metal nanoparticles, Rh, Co, Fe, Pt and their composites with functionalized graphene, RhNPs@f-graphene, Co@f-graphene, PtNP@f-graphene were synthesized and characterized by SEM and TEM techniques. The SEM analysis indicates that the RhNPs are dispersed on f-graphene layers like water droplets on lotus leaf (Figure). The composite RhNPs@f-graphene electrocatalyses hydrogen gas evolution from water containing p-toluene sulphonic acid at an onset reduction potential, E_p , -0.117 V which is much less than that for PtNPs@f-graphene (E_p , -0.380 V) under identical experimental conditions (Figure). The onset potential for CoNPs@f-graphene was observed at E_p , -0.97 V and the FeNPs@f-graphene displayed the onset potential at E_p , -1.58 V. The pure rhodium nanoparticles, RhNPs were also found to be highly efficient electrocatalysts which displayed reduction onset potential at E_p , -0.186 V compared with that of PtNPs at E_p , -0.36 V and that of CoNPs at E_p , -0.98 V. The electrocatalytic experiments also indicate that the RhNPs and RhNPs@f-graphene are stable, durable and they can be recycled in several catalytic experiments. The importance of Wilkinson's metal is recognized as the reduction potentials were much higher in other transition metal nano-electrocatalysts. The mechanism could be the interaction of protons with the Rh sites and reduction to a hydridic species Rh-H⁻ upon application of negative electrode potential followed by interaction with further protons to form hydrogen gas.

Abstract ID: 831

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Bio-inorganic nanomaterials

Keywords: Chitosan, Nanohybrid, Sensors, Anions

Biopolymeric Metal-Azo Nanohybrids as Sensing Material for Toxic Water-Soluble Anions

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Excellent chemo sensors with chitosan functionalized methyl orange (CFMO) metal nanocomposites (CFMO-MNps) have been synthesized by chemical methods and characterized by spectroscopic techniques. These materials displayed efficient selectivity and sensitivity for cyanide and arsenate anions in aqueous media. The electrostatic attraction between the metal induced cationic N,N-dimethylbenzenamine end and the anions provides remarkable colorimetric responses (Fig 1). FT-IR and UV-visible studies confirm the presence of the reacting functional groups. The varying linear orientation to monodispersed distribution of the nanoparticles as revealed by the SEM micrographs support the high degree of sensitivity. The obvious selective color changes can be exploited for real time and on site applications.

Abstract ID: 832

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Micro/Nano-electronics and MEMS

Keywords: smart materials, functional materials, micromechanical response

Time-response limits on vanadium dioxide micrometer-sized actuators

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Research on the performance of micrometer-sized actuators found a new path since the discovery of the effects of solid-to-solid phase transitions in vanadium dioxide thin film coatings on such devices. It was reported that the change in area of the crystallographic planes in VO₂ parallel to the surface of a micrometer-sized cantilever is capable of producing stress levels that generate significant actuation displacements and strain energy densities. Recent advances have focused on increasing different performance parameters such as energy consumption, speed, flexibility, and most recently, wavelength responsivity. However, a clear study on the mechanical time-response, and the electro-thermo-mechanical coupling has not been reported. In this work, we report VO₂-based electro-thermally activated micrometer-sized devices; where the mechanical time-response is described in terms of the electrical input and the thermodynamics of the process. We describe the theoretical limits of speed on VO₂-based actuators using the thermal properties of VO₂, the structural materials forming the device, and its geometry. In the process we use a high-speed camera to correlate the mechanical output to the mechanical input. The results are confirmed by alternative optical-based testing approaches and the theory that explains the process is presented.

Abstract ID: 833 / Poster: 8

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Solar Cells

Keywords: Perovskite solar cells, SnO₂ quantum dots, electron transport layer, air-processed PSCs.

Air-processed perovskite solar cells made with SnO₂ quantum dots

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SnO₂ displays a wider band gap that may decrease absorption of high energy photons by the electron transport layer (ETL), leading to less current loss and greater electron mobility when compared with TiO₂. Therefore, large-scale perovskite solar cells (PSCs) incorporating SnO₂ as the ETL may have a higher stability. SnCl₂•2H₂O in DI water can be self-evolved into SnO₂ quantum dots through the hydrolysis-oxidation process with urea as an additive to accelerate the reaction. The SnO₂ layer can be easily fitted in PSCs by spin coating. The power conversion efficiency (PCE) of the SnO₂-based PSC is as high as 12.5% in the reverse scan with the configuration of FTO/SnO₂/perovskite/CuPc/carbon paste. The active area of the PSCs was 0.1 cm² with a mask. Note that the PSCs were prepared in the air ambient under high relative humidity of 50-55%. This work demonstrates the use of low-cost air-processed PSCs with spin-coated quantum dots as the ETL for enhanced PCE.

Abstract ID: 834

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Solar Cells

Keywords: Perovskite solar cells, hole transport layer, heptane solvent, air-processed PSCs.

Preparation of perovskite solar cells without a hole transport layer in ambient air

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Moisture and oxygen present during preparation of solution-deposited perovskite solar films in ambient air may cause negative impact on the quality of perovskite films. In the present work, solution phase deposition of perovskite thin films in ambient air with humidities of 50-55% was achieved. The perovskite precursor solution was initially mixed with nonpolar solvents such as heptane, which was subsequently heated for film layer self-assembly during solvent evaporation. We found that increasing solvent vapor pressure at elevated temperatures may reduce oxygen and moisture exposure during the perovskite thin film deposition. With this simple thermal evaporation method for thin film deposition without a hole transport layer, the perovskite solar cells were composed with a configuration of carbon/CH₃NH₃PbI₃/porous TiO₂/compact TiO₂/FTO, fabricated under a humid atmosphere of 50% RH and demonstrated a power conversion efficiency of 6.72%.

Abstract ID: 835

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Manufacturing and formation techniques

Keywords: plasticity, UMAT, Dream.3D, Abaqus

A Digital Representation of a Microstructure and Determining its Mechanical Behavior

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Mechanical characterization tests might come with a remarkable cost of time and money for both companies and academics. The inquiry to transform laboratory experiments to the computational media is getting a trend; accordingly, the literature supplies many analytical ways to explain the mechanics of deformation. In our work, we focused on the crystal plasticity finite element modeling (CPFEM) analysis on various materials in various crystal structures to predict the stress-strain curve without tensile tests. For FEM analysis, which we used in this study was ABAQUS, a standard user defined material subroutine (UMAT) was prepared. The geometry of a specimen was created via DREAM 3D software with the inputs of Euler angles taken by Electron Back-Scattered Diffraction (EBSD) technique as orientation, or misorientation angles. The synthetic crystal created with DREAM 3D is also meshed in a way the grains inside the crystal meshed separately, and the computer can realize interaction of inter, and intra grain structures. The mechanical deformation parameters obtained from the literature put into the Fortran based UMAT code to describe how material will response to the load applied from specific direction. The mechanical response of a synthetic crystal created with DREAM 3D agrees well with the material response in the literature.

Wednesday, 21/Aug/2019 4:00pm - 4:12pm

Abstract ID: 836 / FCM: 1

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Applications of Composites

Keywords: Brilliant Green, Pd-Fe/RGO Nanocomposites, Artificial Intelligence, Isotherm Study, Kinetic Study

Decolorization of Brilliant Green in Aqueous Phase by the Ordered Mesoporous Pd-Fe/RGO Nanocomposites Using an Artificial Intelligence Aided Modeling and Optimization

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The ordered mesoporous Pd-Fe bimetallic nanoparticles immobilized on the reduced graphene oxide (Pd-Fe/rGO nanocomposites) were used in the present study for the decolorization of toxic brilliant green (BG) dye in aqueous phase. The decolorization process was modeled and optimized by artificial intelligence (AI) technologies that may revolutionize the human society. AI technologies employed include back propagation neural network-particle swarm optimization (BP-PSO) and back propagation neural network-genetic algorithm (BP-GA) hybrid models. The Pd-Fe/rGO nanocomposites were synthesized by two-step reduction in aqueous phase and then characterized with scanning electron microscopy, X-ray diffraction, N₂-sorption, energy dispersive spectroscopy, Raman spectroscopy, superconducting quantum interference device and X-ray photoelectron spectroscopy. These nanocomposites possessed a Brunauer–Emmett–Teller surface area of 164.1519 m²/g, a single point adsorption total pore volume of 0.4783 cm³/g, a Barrett-Joyner-Halenda adsorption average pore width of 10.8575 nm, and a narrow pore size distribution with a center of 3.47 nm, therefore they belonged to well-ordered mesoporous materials. According to response surface methodology (RSM), batch experiments were carried out to investigate the effect of operational parameters (i.e. initial pH (4–6), initial concentration (400–600 mg/L), contact time (2–8 min) and temperature (25–35 °C)) on the decolorization of BG in aqueous solution. The predictive ability was evaluated for RSM and AI models (i.e. BP-PSO and BP-GA) developed based on the batch experiments. The results indicate that the BP-GA model has a better performance than the other two models. The experimental equilibrium data of BG adsorption onto Pd-Fe/rGO were fitted to the Langmuir and the Friedrich isotherm equations by linear and nonlinear methods. It was seen that the R² value obtained was better from the linear fitting. The adsorption equilibrium follows Langmuir isotherm and the maximum adsorption capacity of Pd-Fe/rGO was 3333.33 mg/g. Three kinetics models including pseudo-first-order, pseudo-second-order and Elovich equations were also utilized to examine the BG decolorization process. It was found that the pseudo-second order kinetic model (R² 0.9989) could satisfactorily describe the removal kinetics data. In addition, thermodynamic studies reveal that the adsorption of BG was spontaneous and endothermic with enthalpy and entropy values of 0.2323 kJ mol⁻¹ and 0.0322 kJ mol⁻¹ K⁻¹, respectively. Overall, these mesoporous nanocomposites have the advantages of large specific surface area, fast decolorization, high

adsorption capacity for BG and optimization of the removal process with the AI technologies was successful.

Abstract ID: 837

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

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

Keywords: Electronic; Heterostructures; Optical; Skutterudites; Two-dimensional WSe₂ density functional theory calculation

DFT Study of Skutterudite CoSb₃ and In_{0.2}Co₄Sb₁₂ Thermoelectric Heterostructures with 2D-WSe₂

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The research on thermoelectric energy generating materials has gained interest in improving efficiency of thermoelectric materials, which is quantified by the dimensionless figure of merit (zT) = $S^2\sigma T / (k_e + K_l)$, where S , σ , T , k_e and K_l are the Seebeck coefficient, electrical conductivity, temperature, electronic thermal conductivity and lattice thermal conductivity, respectively. Different approaches, such as doping heavy atoms within complex structures, anisotropic thermal vibrations, atomic disorder “rattlers” filled cage structure, defects and grain boundary scattering, and the superlattice structures are being employed to lower the lattice thermal conductivity by scattering acoustic phonons. Recently, two-dimensional WSe₂ transition-metal dichalcogenides have been used for novel electronic devices. However, its influence on the electronic and optical properties of thermoelectric Skutterudite CoSb₃ and In_{0.2}Co₄Sb₁₂ is unknown. Despite the increased potential of energy conversion obtained by doping CoSb₃ with indium, further theoretical study is necessary to understand the origin of this enhancement. Heterostructures of hybrid WSe₂/CoSb₃ and WSe₂/In_{0.2}Co₄Sb₁₂ are investigated in this study using a density functional theory calculation. The electronic structure, energy, geometry optimization and optical properties are analyzed for the individual components in the heterostructure. The obtained results show that pure CoSb₃ has a bandgap of 0.456 eV, and In_{0.2}Co₄Sb₁₂ has a zero bandgap, while the calculated bandgap for WSe₂ is found to be 1.482 eV. The heterostructures show an exceptional absorption in the infrared region where the heat energy mainly dominates. The charge transfer study indicates a built-in potential at the interface, which ensures easy separation of charge generated carriers and thus, improved the thermoelectric performance.

Wednesday, 21/Aug/2019 6:00pm - 6:12pm

Abstract ID: 838 / FBB-2: 11

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Drug delivery/controlled release

Keywords: Nitric oxide, Graphene oxide, Fluorinated poly(ethylene glycol), Anti-bacterial activity, Escherichia coli, Staphylococcus aureus.

Fluorinated poly(ethylene glycol)@graphene oxide platform for nitric oxide gas delivery system and their antibacterial activity

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Nitric oxide (NO) is an endogenously synthesized molecule which can mediate numerous physiological processes[1,2]. In the meanwhile, exogenously, NO exerts vasodilator, tumoricidal and antibacterial effect but its usefulness is limited due to high reactivity, amount dependency and unavailability of the carrier that can efficiently encapsulate the gas[3,4]. In response to the needs for such bioactive gas in therapy, we prepared NO conserving platforms of graphene oxide (GO) and its composite with fluorinated poly(ethylene glycol) (F-PEG) by non-covalent functionalization. The shape and size of GO and F-PEG@GO confirmed from transmission electron microscope and dynamic light scattering technique were sheet measured 207 and 250 nm, respectively. Coexistence of GO and F-PEG in a composite was confirmed from Fourier transform infrared absorption (FTIR) spectra, Raman scattering spectra, thermogravimetric analysis, and X-ray diffraction (XRD). The doping amount of NO in GO and F-PEG@GO were analyzed using Griess assay methods. The conserved NO gas was more for F-PEG@GO than for GO and decreased with time due to either the oxidation of NO to NO₂ or the release of NO from the carrier. The conservation of NO gas on carrier was related to the surface area of the carrier and confirmed by FTIR spectra, XRD and XPS. The anti-bacterial effect of NO gas from doped GO and F-PEG@GO were examined against Escherichia coli and Staphylococcus aureus. NO gas preserved in F-PEG@GO exerted higher anti-bacteria effect than GO and more effective against S. aureus than E. coli. Thus, the F-PEG-coated GO composite was effective for NO gas conservation and anti-bacterial effect superior to GO.

Key words: Nitric oxide, Graphene oxide, Fluorinated poly(ethylene glycol), Anti-bacterial activity, Escherichia coli, Staphylococcus aureus

Abstract ID: 839

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Porous and cellular materials

Keywords: Bituminous Coal, Carbonization, Fractal, Small Angle X-Ray Scattering, Synchrotron Radiation

Small angle X-ray scattering study on the fractal structure of solid products of bituminous coal at different carbonization temperatures

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Carbonization is one of the main methods for comprehensive utilization of bituminous coal. Bituminous coal and its solid products from carbonization, namely char and coke, have complex pore structure, which can be characterized by fractals. We performed a study on the fractal structure of the solid products prepared from the bituminous coal of Shuiyu mine in Shanxi Province, China, at different carbonization temperatures (25°C~1000°C) by synchrotron radiation small angle X-ray scattering (SAXS). The results show that all samples present surface fractal structure from room temperature to 1000°C. The change of fractal dimension versus temperature indicates that the carbonization of the bituminous coal occurs in stages: physical desorption stage from 25°C to 200°C; lignite softening stage from 200°C to 500°C; char formation stage from 500°C to 800°C; and coke formation stage 800°C to 1000°C. The change of fractal dimension well reflects the change of physical structure of pores caused by chemical reaction during carbonization.

Abstract ID: 840 / Poster: 9

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Structural, Electronic, Optical and Magnetic Properties

Keywords: Pulsed Laser, Graphene, Nano Inductor

Pulsed Laser Scribed Graphene/Polymer composites: A Potential Route to Print on-chip Carbon Nano-Coil Inductors

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There is great interest in so-called nanoscale electronic devices due to the furious rate of device miniaturization, but so far, there has been little development in the way of nano-scale coil inductors. Methods exist for creating conductive polymer coils, but their isolation and characterization for device applications is beyond current technology available, so simpler fabrication techniques are needed. In this work we demonstrate a technique consisting of the pulsed laser scribing of a polymer/graphene oxide film composite which results in a large inductive effect. We attribute this behavior to the formation of inductive carbon nano-coils composed of polyacetylene chains linked by pi-pi interactions to reduced graphene oxide flakes.

Acknowledgement: This work is supported by

NSF HBCU UP Award # 1719425,

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Thursday, 22/Aug/2019 5:18pm - 5:30pm

Abstract ID: 841 / FESC-2: 17

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Magnesium Ion Batteries

Keywords: Mg-ion battery anode, self-healing, operando X-ray scattering, solid-liquid phase transition

A Long Cycle-Life and High-Rate Magnesium-Ion Battery Anode Enabled by Self-Healing through Near-Room-Temperature Solid-Liquid Phase Transition

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The growing popularity of lithium-ion batteries has raised a serious concern about the long-term supply of these batteries, since lithium and cobalt resources used are becoming more expensive due to demand, and the global cobalt market heavily depends on the supply from countries with high geopolitical risks. Therefore, scalable alternatives battery technologies are desirable to reduce the dependence on lithium and cobalt. Over the past few years, magnesium-ion batteries have been the subject of intense research as an alternative to lithium, owing to the various advantages of magnesium including the abundance of magnesium resources for large-scale applications. Nevertheless, progress toward practical magnesium-ion batteries has been impeded, partly by the absence of suitable electrolytes that are compatible with magnesium metal used as the negative electrode. Typically, common salts and organic solvents combinations similar to those used in lithium-ion batteries yield a magnesium-ion-blocking passive film on the magnesium metal negative electrode. A promising way to circumvent this electrolyte issue is through the use of alloy-type anodes as the negative electrode instead of magnesium metal. However, state-of-the-art alloy-type magnesium-ion battery anodes can only be reversibly cycled up to 200 times with acceptable capacity retention 1. Such a cycle-life is far below the thousands of cycles required for practical battery applications. In this talk, I will present a novel high-performance alloy-type magnesium-ion battery anode which we have developed, which can be reversibly (de)magnesiated at the C-rate of 3C over 1000 cycles with excellent capacity retention. This exceptional performance is thanks to the self-healing property of the active electrode material, which undergo solid-to-liquid phase transition when the cell operate around 30-40oC. Operando X-ray scattering techniques were used to demonstrate this self-healing property in real-time during magnesiation and demagnesiation.

Abstract ID: 842

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Applications of Composites

Keywords: polymer hybrid nanocomposites, synergistic effect, mineral nanofillers, halloysite nanotubes, dental applications

Acrylic based nanocomposites containing hybrid system of mineral nanofillers for dental applications

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Acrylic materials (in particular methyl methacrylate or poly(methyl methacrylate) (PMMA)) are widely used in many industries, such as automotive and construction, and fields, such as medicine or cosmetology [1]. Moreover, they can be used both independently and in a system with different fillers to form composites or nanocomposites if at least one of the dimensions of the filler reinforcing phase does not exceed 100 nm. HNTs are naturally occurring polymorph of kaolinite with a dominant hollow tubular morphology, which, due to their properties and origin, show potential biocompatibility for applications in medicine. The present study involved research related to the selection of the material with improved functional properties that can be used for dental prostheses [2]. An innovative system of nanofillers, that differ in shape, by means of gelatin-modified halloysite nanotubes (HNTs-g) along with silane-coupled aluminum trihydrate (ATH-sil) was prepared, in order to observe a synergistic improvement of acrylic material (methyl methacrylate with methyl methacrylate monomer (MM/mMM)). Selected mechanical properties of manufactured nanocomposites, along with utilitarian properties, like hardness, buffer solution absorption, and abrasion resistance, along with a fall test from the height of finished products have been discussed. Moreover, the study of the biofilm formation on the surface of dental prostheses confirmed the occurrence of a synergistic improvement of properties and the legitimacy of using modified mineral nanofillers in the form of a hybrid system [2].

Abstract ID: 843

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Magnetic film

Keywords: epitaxial oxide films, uniaxial strain, magnetron sputtering

Helium doping in manganite films via. magnetron sputtering in He-mixed atmosphere: A simple strategy for uniaxial strain engineering

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Strain engineering in oxide films has been extensively studied since the discovery of high-temperature superconductivity in copper oxides. However, most of previous work was confined to the in-plane biaxial strains by using substrates with various lattice parameters. Recently some authors demonstrated independently tuning the out-of-plane lattice of manganite films through He⁺-ion implantation. To get around the usage of specialized ion implantation equipments, in this work we implement the He-doping by using the routine magnetron sputtering technique in an atmosphere mixed with He gas. La_{0.7}Ca_{0.3}MnO₃ (LCMO) films on single crystal SrTiO₃ substrates were chosen as the prototype, which suffer biaxial tensile strain in the film plane. Due to the positive Poisson's ratio of the oxide, the tensile strained LCMO films inevitably possess a shorter out-of-plane (c) lattice parameter, accompanying with a suppressed ferromagnetic transition temperature (TC). Our first approach to stretch the c-axis was adding He gas in the conventional Ar–O₂ mixed sputtering atmosphere. With increasing the He gas ration to around 15%, it is found that the c-axis increases from 3.823 to 3.845 Å, accompanying with an increase of TC from 260 to 280 K. Thermal stability experiments provide further evidence for the He-doping in the films. Then we speculated two possible He-doping processes during the He-co-sputtering deposition: One is He⁺-ion implantation on the LCMO cathode target, and the other is He atom adsorption on the film/substrate surface. To indentify the two possibilities, we performed glow discharge of He gas before conventional sputtering deposition in the Ar–O₂ mixed atmosphere, and repeated injection of He gas between several conventional sputtering depositions, respectively. While the LCMO/STO films obtained through the latter way change little, the films deposited after He glow discharge display a substantial increase in both the c-axis and TC, revealing that the He⁺-ion implantation into the cathode target plays a key role in the He-doping process. Based on this finding, we tried to implant He⁺-ions into the as-grown films by directly placing them on the cathode in He glow discharge. The He⁺-ion-treated film shows an even larger c-axis ~ 3.851 Å, as well as a higher TC ~ 290 K. Finally, the overall conclusion is: magnetron sputtering in the He atmosphere is a simple method for He-doping in oxide films, which in turn leads to an effective control on the uniaxial strain in the films.

Wednesday, 21/Aug/2019 4:00pm - 4:12pm

Abstract ID: 844 / FBB: 1

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Advances in Enzymatic and Non-Enzymatic Biosensors

Keywords: Biosensors, Nanopore, ADAMs Enzymes, Metal ions

Enzyme assisted nanopore detection of Zn(II) ions

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Nanopore sensing is an emerging analytical technique, which has received extensive attention due to its high sensitivity and versatility. Biological protein ion channels are especially appealing as nanopore sensing elements due to several advantages. For example, they offer atomic-precision structural reproducibility, and have similar pore sizes as those of many biologically important analyte molecules. Nanopore sensors are able to detect analyte molecules rapidly and sensitively without requiring labels or tags, and will have a great potential for portable application.

By taking advantage of ionic strength and salt gradient, and monitoring the enzymatic cleavage reaction between a substrate peptide and zinc dependence enzyme in a nanopore, we developed a label-free metalloproteinase enzyme based nanopore sensor for the rapid detection of zinc ion. The sensor was highly sensitive and selective: nanomolar concentrations of Zn(II) ion could be detected within minutes, whereas structurally similar transition metals such as Ni(II), Hg(II), Cu(II), and Cd(II) did not interfere with its detection. The developed strategy in this work may find potential applications in environmental monitoring and medical diagnostics.

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Abstract ID: 845

Symposium 3: Functional Catalysis (FC)

Poster Presentation

Topics: Catalysis for Chemical Synthesis

Keywords: Palladate Magnetic Carbon Quantum, Hybrid of Cyclodextrin Nanosponges, Hydrogenation

Palladate Magnetic Carbon Quantum Dot Immobilized on the Hybrid of Cyclodextrin Nanosponges and Bell-pepper Derived Biochar: A versatile Catalyst for Promoting Hydrogenation Reaction

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Palladate Magnetic Carbon Quantum Dot Immobilized on the Cyclodextrin Nanosponges-Bell pepper Derived Biochar hybrid: A versatile Catalyst for Promoting Hydrogenation Reaction

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Char is a non-graphitizable material and is defined as a product from carbonization process of carbon precursors without achieving a fluid state in the process. Popularly, char derived from biomass such as wood and waste is known as biochar. Because of these advantages, biochar has great potential to be used in the fields of heterogeneous catalysis, pollution control, and etc. [1] In the other cases of carbons, carbon quantum dots (CQDs) are a novel class of carbon nanomaterials with sizes below 10 nm. At first, CQDs were found through purification of single-walled carbon nanotubes with preparative electrophoresis in 2004 [2]. CQDs have slowly become a valuable structure in the nano carbon domestic, because of being high solubility, non-toxic and low-cost nature. Furthermore, it is worth mentioning that CQDs have an advantage of unique electron transfer, indicative of a great potential as a heterogeneous catalyst. In the following of our interest in the above mentioned achievements [3-5] we focused on studying the catalytic performance of palladate magnetic CQDs immobilize on cyclodextrin nanosponges-biochar hybrid for the hydrogenation reaction of nitrobenzene. In this regard, herein we wish to report our effective achievement on the preparation of the heterogeneous catalyst, which was prepared through immobilization of Pd and Fe₃O₄ NPs on CQDs followed by incorporation of cyclodextrin nanosponges-bell pepper derived biochar (CDNS-Biochar). Then, the catalytic performance of the catalyst was investigated for promoting hydrogenation reaction of nitrobenzenes to afford anilines in high yields and short reaction times. Moreover, the catalyst could be recovered and recycled for ten reaction runs with slight loss of leaching of Pd and Fe species.

Key Words: Biochar, CQDs, Heterogeneous catalyst, Hydrogenation.

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Thursday, 22/Aug/2019 11:12am - 11:24am

Abstract ID: 846 / FLNM-2: 2

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Computational modeling and simulation of low dimensional, nano and 2D materials

Keywords: Perovskites, Buckingham Potential, Molecular Dynamics, LAMMPS

A Molecular Dynamics Study of Perovskite Structure Crystal Correlations

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The demand on new and highly efficient energy conversion systems and many other advanced applications have suggested the Perovskite family to be an important future candidate material. Though a lot of work has been done in order to understand and simulate their structure, further investigation is still needed. The understanding of their structure and electrochemistry is limited by the complexity of experimental work. Consequently, the development and enhancement of computational methods including molecular dynamics and quantum chemical calculations is one of the main issues regarding the optimization of perovskites.

In this work, different interatomic potential functions are investigated to analyze the structure of perovskites in intention to simulate nondegradable stable configurations through the application of Molecular Dynamics via LAMMPS open source code. Such equilibrium configurations would lead to deduction of mechanical and thermal properties and to building a platform for adapting the different types of perovskites to enhance their technological aspects. The most well-known potential functions used in literature are Buckingham potential, Vashishta-Rahman (VR) and Lennard-Jones (LJ) potentials.

Specifically, in this study; Buckingham potential is compared with VR and LJ potentials in representing different perovskites. The VR interaction potential was previously proven to be the most effective for describing the phase changes of perovskites and to match the experimental observations [1]. It was also proven in previous studies that the radial distribution function (RDF) undergoes essential changes when replacing LJ with VR [2]. However, according to the findings of this study, Buckingham potential is shown to produce closer results to VR than LJ. Consequently, densities, melting points and stress-strain curves of CaTiO₃ and BaTiO₃ were achieved using Buckingham representation with error less than 1% when compared with reported data in the literature. The specifics of the atomic pair re-organization due to interatomic potential alterations illuminate on the critical role of potential function representation of the perovskite systems.

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Abstract ID: 847

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Hybrid cells for energy harvesting

Keywords: Dual-functioning multiple-quantum well diode, subwavelength vertical-structure, simultaneous emission-detection phenomenon

Dual-functioning subwavelength vertical-structure multiple-quantum well diode

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We propose for the first time a dual-functioning subwavelength vertical-structure multiple-quantum well diode (MQW-diode). Subwavelength vertical-structure MQW-diodes are implemented on a 2-inch metal-based bonded III-nitride-on-silicon wafer [1]. As shown in Fig. 1, thick III-nitride films are thinned without hard mask to a thickness d , which is smaller than the wavelength λ (450 nm) of the generated light [2]. Therefore, light emission in the in-plane direction can be inhibited when the forward voltage is applied to the MQW-diode to generate light and thus, the light will go right through the vertical-structure MQW-diode without getting lost. Especially, the MQW-diode exhibits the simultaneous emission-detection phenomenon because there is an overlap between its emission and detection spectra [3]. As a result, the subwavelength vertical-structure MQW-diode can generate and sense light at the same time, and the superimposed signals can be extracted by integrating an external control circuit. The fabricated MQW-diode experimentally demonstrates full-duplex spatial audio communication, opening promising approaches toward a variety of novel applications.

Thursday, 22/Aug/2019 8:12am - 8:24am

Abstract ID: 848 / FESC: 2

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Oral Presentation

Topics: Sodium Ion Batteries

Keywords: Na Cathode, Interface Engineering, Energy Storage

High-Rate and Long Cycle-Life of Bulk $\text{Na}_{2/3}[\text{Ni}_{1/3}\text{Mn}_{2/3}]\text{O}_2$ Sodium-ion Battery Cathode Enabled through Structural Inclusions

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Recently, sodium-ion batteries (SIB) have been considered a promising alternative to lithium-ion batteries, due to the abundance of sodium resources (Na is the Earth's 6th most abundant element, while Li is 33rd) and its low extraction costs. Among various cathode candidates, the layered oxides NaTMO_2 (TM=3d transition metal elements and their mixture) can accommodate sodium ions through the intercalation mechanism, but suffer from major limitations including a poor rate capability and short cycle life. We have developed a novel bulk $\text{Na}_{2/3}[\text{Ni}_{1/3}\text{Mn}_{2/3}]\text{O}_2$ structure containing inclusions, which, exhibits an unprecedented rate capability with roughly 50% capacity retention at 50C, and a remarkable long-term cycling stability with 95% capacity retention after 1000 cycles at 5C. During this talk, I will present our new results and elucidate the mechanism through which the cycling performance of the novel materials system is enhanced.

Abstract ID: 849

Symposium 2: Functional Composite Materials (FCM)

Poster Presentation

Topics: Composites in Innovative Applications

Keywords: Multiple-quantum-well diode, confined optical mode, simultaneous emission-detection phenomenon

225-nm-thick vertical structure multiple-quantum-well diode

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We propose and fabricate an ultrathin multiple-quantum-well diode (MQW-diode) to reduce optical waveguide modes inside thick device [1]. A 225-nm-thick vertical-structure MQW-diode is implemented on a 2-inch III-nitride-on-silicon platform [2, 3]. Thick III-nitride films are thinned to 225 nm without hard mask, and one 10- μm -wide and 155- μm -long waveguide impinges on the MQW-diode to characterize the in-plane light coupling between the MQW-diode and the waveguide, as shown in Fig. 1. The fabricated 225-nm-thick MQW-diode works well and exhibits a dominant electroluminescence peak of 411 nm. Because the MQW-diode thickness d is smaller than the emission wavelength λ of 411 nm, confined optical modes are inhibited and the in-plane light propagation can not exist. As a result, no scattered light spot is observed at the waveguide end facet and all light emission finally goes through the device without getting lost. The MQW-diode also can function as a photodiode to detect light. In particular, the simultaneous emission-detection phenomenon of the MQW-diode that is caused by the spectral overlap between its emission and detection spectra is experimentally demonstrated [4].

Abstract ID: 850

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Thin Films in Biological and environmental Applications

Keywords: Whey protein isolate, Pullulan, Maillard reaction, Barrier properties, Antioxidant activity

Effect of Maillard reaction on barrier and antioxidant properties of whey protein isolate/pullulan based edible films

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This study used orthogonal experiments to optimize the barrier properties and antioxidant properties of the Maillard reaction for edible films based on whey protein isolate, sodium caseinate and pullulan. The films were prepared by using different ratios of whey protein isolate, sodium caseinate and pullulan, and the films were heated under dry conditions at different pH and temperature for 24 hours to induce Maillard reaction. Color changes and browning index measurements were used to pursue the MR kinetic. Fourier transform infra-red (FTIR) spectra confirmed that Maillard reactions occurred between whey protein isolate, sodium caseinate and pullulan. The performance parameters of these modified films were measured respectively, such as mechanical properties, optical properties, barrier properties to gas and water vapor, antioxidant activity, degree of crosslinking, water solubility, molecular structure, etc.. The results showed that the Maillard reaction effectively reduced the oxygen transmission rate, water solubility of the films, and increased the tensile strength and percentage of elongation at break. The in vitro antioxidant activity of composite films modified by Maillard reaction was studied by using total antioxidant activity and the reducing power. The antioxidant capacity of the films is significantly enhanced. These results indicated that composite whey protein isolate-sodium caseinate-pullulan films modified by Maillard reaction are expected to be used in food edible packaging materials to protect products from oxidation.

Abstract ID: 851**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Alloy anodes

Keywords: Operando TEM, Nanoporous Metals, Energy Storage

Operando TEM Investigation of Lithium Storage Mechanisms in Nanoporous Alloy-Type Lithium-Ion Anodes

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High-capacity alloy-type lithium-ion battery anodes can undergo large volume changes (~300%) during lithiation.¹ The resulting stresses can cause pulverization and delamination of active material from the current collector, rendering it electrochemically inaccessible. Previous work demonstrated that nanoporous electrode materials, consisting of bicontinuous network of nanoscale solid ligaments and pores, have improved cycling performance compared to their bulk counterparts. Currently, it is hypothesized that this volume change is minimized due to a buffering mechanism in which the ligaments expand while the pores shrink, resulting in a smaller lithiation-induced net volume change.¹ In an attempt to verify this hypothesis, Detsi and his colleagues have used synchrotron-based transmission X-ray microscopy (TXM) to image these volume changes and found that nanoporous Sn grains accommodate the lithiation-induced volume changes better than dense Sn.² However, the TXM is only able to accurately probe the volume change in sub-micrometer sized Sn grains. In order to confirm the above hypothesis, one needs to observe the structural evolution of the nanoscale pore-ligament structure of 3D nanoporous alloy-type Li-ion battery anodes during galvanostatic cycling. This will be accomplished through the use of transmission electron microscopy (TEM). A Hummingbird Scientific electrochemistry TEM specimen holder will be used to facilitate the lithiation and delithiation of a “nanobattery³” while different TEM techniques are performed simultaneously. Through this methodology, this experiment will be able to address fundamental questions involving structural changes in nanoporous alloy-type lithium-ion battery anodes during lithiation / delithiation cycles.

Key Words: Operando TEM, Nanoporous Metals, Energy Storage

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Abstract ID: 853

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: Thermal energy storage, infrared stealth, Microcapsule, thermal property

Infrared stealth and phase change microcapsules based on stearic acid and nano-iron

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Micro-encapsulated phase change materials are playing an eye-catching role for easing the energy crisis in recent years, but most of them in current studies only have the function of thermal storage and temperature control, which limits their further application. In this study, a dual-function micro-encapsulated phase change material with the functions of thermal storage, temperature control and infrared stealth was designed by in-situ polymerization with stearic acid as core material, calcium carbonate as hybrid wall material and nanocrystalline iron as modified material. The thermal properties of the samples were characterized by scanning electron microscopy, Fourier transform infrared spectroscopy, thermogravimetric analysis and differential scanning calorimetry. On the other hand, infrared stealth characteristic of samples were analyzed by infrared emissivity and infrared photograph. The results show that the solidification temperature of the samples are in the areas of 57°C – 65°C and the melting temperature are in the areas of 60°C – 75°C. The melting and solidifying enthalpies of the samples reached up to 139.21 J/g and 134.84 J/g, respectively. The optimum encapsulation ratio of the calcium carbonate to the stearic acid is about 79%. In addition, the infrared emissivity are in the areas of 0.39 – 0.71. The microcapsules synthesized in this study have dual-functional properties and can provide a new way to achieve both thermal energy storage and infrared stealth in some high-tech fields.

Key Words: Thermal energy storage, infrared stealth, Microcapsule, thermal property

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Abstract ID: 854

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Environmental Catalysis

Keywords: Catalytic Diesel Particulate Filter, Air Regeneration, Heavy-Diesel-Engine-Vehicle

Research of the Pollution Control Technology of the Particulate Matter for Diesel Vehicle

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The diesel exhaust pollutants have a high concentration from among the soot. The study is to investigate the fundamental chemistry and material microstructures of air regeneration for Catalytic Diesel Particulate Filter (CDPF), and thus synthesizing catalyst can removal pollutant under the diesel engine emission temperature. The model soot for monolithic-honeycomb DPF, Pt/Al₂O₃-cordierite, is diesel-containing soot extracted from the heavy-diesel-engine-vehicle emission control system. The air regeneration was then performed by flowing appropriate air with temperature ramping from room temperature to 500 °C. Time-varying CO₂ concentration in the effluent was used to evaluate the effect of catalytic regeneration. The regeneration testing results indicated that soot combustion rate was only slightly increased by the impregnation of Pt on cordierite, whereas that was greatly increased when the deposition of Al₂O₃ on cordierite, prior to the introduction of Pt. The regeneration efficacy was further improved via the coating of CeO₂ into the face of catalytic. Moreover, the amount of Pt used in catalytic DPF preparation reduced by the addition of much cheaper Ag. The catalytic performance test results suggested that Pt may play an important role in decreasing ignition temperature, while Ag assists Pt in increasing soot combustion rate. This study offers the path to improve the catalytic performance of commercial products.

Abstract ID: 855

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Thin Film Growth & Epitaxy

Keywords: Thick film screen printing, Chemical replacement reaction, Al, Cu, Ni, conductivity

A novel method to fabricate a thick film Cu electrode fired in air

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Thick film screen printing is mature, cost-effective manufacturing processes in micro-electronic industries. The thick film conductor paste has been applied to electronic products extensively, and developing a conductor sintered in air to have both low cost (low materials cost and low process cost) and high electrical conductivity are main object

The thick film conductors paste applied the most widely are Ag and Cu due to having high conductivity. Ag paste can be sintered in air to have high conductivity, but its disadvantage is the overly high cost. Contrarily, though Cu thick paste has a low materials cost, Cu thick film paste must be sintered in reducing atmosphere to obtain a high conductivity, leading a high process cost.

A novel method for fabricating the base metal or alloy electrode such Cu, Ni, or CuNi in air atmosphere for high temperature firing has successfully developed based on thick film screen printing Al pastes and reduction-oxidation substitution reaction. The first thick film screen printing Cu electrode with high conductivity ($>10^{-6} \Omega$), which is comparable to thick film Ag electrode has been successfully made in air firing instead of reducing atmosphere firing.

To make a excellent Cu electrode substituted for thick film Al electrode, the Al paste with high solid content and big particle size of Al powder and CuSO₄ solution with low pH、high temperature, proper soaking time are all positive parameters.

Abstract ID: 857

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Oral Presentation

Topics: Natural biomaterials

Keywords: Hemicellulose Extraction, Hemicellulose modification, Hemicellulose functional properties, Biomaterials, Biocomposites

Diversifying structural and functional properties hemicelluloses through manipulation of pretreatment, extraction and modification conditions to produce advanced biomaterials and biocomposites

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Hemicellulose is one of the major components in the plant cell wall matrix that is present in diversified forms depending on the feedstock. The complex structure associated with the hemicelluloses is both an advantage and a limitation during extraction and modification for different applications. In this paper, results from hemicellulose pretreatment, extraction and modification experiments to tailor make the functional properties of the hemicelluloses to produce advanced biomaterials for application as additives in baking, surface modifiers and coating materials in papermaking, as slow release devices in bioactive agents' targeted delivery, and as a reinforcements, fillers and matrix materials in biocomposites. The hemicelluloses were extracted from feedstocks including, wheat straw, wheat bran, Eucalyptus grandis, bamboo, Pinus patula, sugarcane bagasse and oat spelt. The modification of the hemicellulose structures and compositions were performed using specialty enzymes that target the removal of side chains and chemical methods. Hemicelluloses that were extracted from wheat bran under conditions that resulted in degree of polymerization (DP) above 4 and were substituted with arabinose side groups replaced up to 2.5% of flour used in baking without compromising the physical properties including bread volume and weight of standard bread. In addition, hemicelluloses that were extracted from the feedstocks and were treated with enzymes that specifically remove the arabinose and glucuronic acid side chains, increased the affinity of the hemicelluloses to cellulosic materials, thus modifying their surface properties based on the surface charge that was measured by zeta potential. Furthermore, the removal of the side chains resulted in the formation of nano-hydrogels that functioned as encapsulation and delivery devices for horseradish peroxidase enzyme and Gallic acid. The manipulation of the pretreatment of the feedstocks, and hemicellulose extraction and modification conditions, tailor made the degree of acetylation of the hemicelluloses, thus influencing its performance in biocomposite with cellulose based materials, which attained multiple functionalities either as absorbent materials or as hydrophobic material, properties that influenced the functional properties of the biocomposites.

Abstract ID: 858

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Poster Presentation**

Topics: Liquid electrolytes, ionic liquids, polymer electrolytes

Keywords: Anode freeLi metal battery; shielding effect; NMC; coulombic efficiency

Enhanced performance of anode free lithium metal battery: Understanding the effect of electrolyte additives in carbonated electrolyte

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Realizing anode free Lithium metal battery (AFLMB) is a promising approach to get higher energy density and easily processed materials¹. However, the uncontrolled lithium deposition during lithium plating/stripping on copper current collector results in dendrite growth and low coulombic efficiency^{2, 3}. Herein, we report the use of electrolyte additive to boost the coulombic efficiency and cycle life of AFLMB using Cu//NMC (333) cell configuration. This battery possesses capacity retention of ~40% after 50 cycles in the presence of additive compared to ~40% after only 15 cycles in the absence of additive. The average coulombic efficiency of Cu//NMC and Cu - Li cells after 50 cycles are 96.50% and 96.82% respectively while it is 91.32% after only 35 cycles in the Cu//NMC cell and 88.28% after 51cycles in Li - Cu cell without additive. The SEM results also show smooth plating/stripping process of lithium. These achievements are stemmed from the comparatively new SEI components formed from the reductive decomposition of anions and the electrostatic shielding effect of cations on the initial growth tip of the protuberances.

Abstract ID: 859

Symposium 6: Functional Thin Films (FTF)

Poster Presentation

Topics: Superconducting Thin Films

Keywords: Atomic force microscopy, Microstructure, Surfaces, Thin films, Superconductors

Vortex manipulation with dots and antidots on superconductivity of REBa₂Cu₃O_{7-δ} films growth by trifluoroacetate metal organic deposition method

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Vortex manipulation with pinning structures is a promoting technique for preparing high quality two-dimension and three-dimension epitaxial films. Through introducing dots and antidots on substrates, a valied method for enhancing superconductor property of REBa₂Cu₃O_{7-δ} (RE, rare earth) thin films with a trifluoroacetate metal organic deposition (TFA-MOD) method is introduced. Dots and antidots in sub-micron size can provide controlled vortex motion. By this vortex manipulation technique, the critical current density J_c and onset transition temperature $T_c(\text{onset})$ of the traditional superconducting REBa₂Cu₃O_{7-δ} thin film can be effective improved. In addition, apparent variation of stress stress occurred in thin film growth by the residual stress measurements. This paper provides a competitive method and theoretical guidance for the effective improvement of superconductivity in REBa₂Cu₃O_{7-δ} thin films.

Abstract ID: 860

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Optical, electrical and magnetic properties of thin films

Keywords: Selective absorber; PVD sputtering; Optical properties; Microstructure; TiNi; Ti, Ti₂O, Al, Al₂O₃

Optical Properties and Microstructure of Ti, TiNi and Al Thin Films before and after Oxidation

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Previous studies [1] aiming at developing air-stable high temperature solar selective surfaces have suggested that the oxidation of TiN at 450 °C results an oxide layer of about 20–30 nm after only a few minutes of heat treatment with oxygen. Since, the thickness of the oxide layer is comparable to the thickness of the absorbing layer of the solar thermal selective absorbers, oxidation was suggested as a candidate process to obtain selective solar layers. In this work, the effect of air- oxidizing of as- deposited Ti, TiNi and Al layers on their optical absorbance and emittance is studied, aiming to develop ceramic–metal composites [2]. This would employ structures consisting of combined metallic and oxides nature. In this work, a thin layer of Al, Ti and TiNi is obtained by using RF magnetron sputtering on a stainless-steel substrate, followed by oxidation at 400°C and 800°C for four and one hours, respectively. The optical properties of the thin films were characterized by spectrophotometer, and Fourier transform infrared spectroscopy. The morphology, topography, and structure were studied by scanning electron microscope, atomic force microscope, and X-ray diffraction. The results showed that in the as-deposited state, the Ti thin film recorded the highest optical absorbance of about 90% with an emittance of 1.8%. After oxidation at 400°C, the thin films recorded significant change in their optical properties; the TiNi thin film showed the highest optical absorbance and lowest emittance of 95.3% and 0.1%, respectively. It was also shown that after oxidation at 400 °C, the deposited layers changed their behavior to show a selective absorbance pattern instead of the flat pattern for all wave lengths, with decreased emittance values in the infrared wave length range. The formation of TiO₂ through the oxidation process of both the TiNi thin film as well as Ti thin film at 800°C was illustrated. The Al thin film showed the lowest optical properties in as-deposited and oxidized states.

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Abstract ID: 861

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Poster Presentation

Topics: Advances in the Synthesis and Characterization of low dimensional, nano and 2D materials

Keywords: flake graphite, graphene, oxide, large size, two-step

Preparation of graphene oxide and graphene by two-step oxidation

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In this paper, graphene oxide and graphene were prepared by using flake graphite with the large size about 300um as raw carbon material by implying two-step oxidation. In the first oxidation step, the inter layer of graphite was opened and the graphite was oxidized and modified with functional groups, such as HSO₄⁻ and SO₄²⁻. In the second oxidation step, the residual unoxidized graphite was oxidized and modified with oxygen-containing groups. Results reply that the obtained graphene is consist of few layer graphene with the ID/IG of 1.52. Meanwhile, the obtained graphene has large specific area of 576.06 m²/g and high electrical conductivity of 19.98 S/cm.

Thursday, 22/Aug/2019 4:39pm - 4:51pm

Abstract ID: 862 / FESC-2: 14

**Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)
Oral Presentation**

Topics: Nanostructured materials for advanced batteries

Keywords: Nanoporous Metals, Atomic Layer Deposition, Energy, 3D Nanocapacitor

3D Nanoporous Conductor-Insulator-Conductor (CIC) Capacitor

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Traditional energy storage devices use a two-dimensional (2D) geometry in which materials are sandwiched between positive and negative electrodes, providing power to an external load on demand. Unfortunately, this tried-and-true geometry cannot satisfy the increasing market demand for energy dense, high-powered, and miniaturized energy storage materials. In a three-dimensional (3D) configuration, energy storage materials can be interwoven in a third dimension to dramatically increase the specific surface area and reduce the overall macroscopic dimension to account for miniaturization while maintaining the desired nanoscale dimension for optimal functionality. State-of-the-art 3D energy storage and conversion systems are based on interdigitated columnar arrays which utilize templates that act as scaffolds for ALD or carbon nanotube growth.^{1,2} In this presentation, I will discuss our work on another 3D configuration, wherein we use high surface-area-to-volume ratio nanoporous metals as the substrate for atomic layer deposition (ALD) of dissimilar metal oxides to create a fully functioning thin film 3D Conductor-Insulator-Conductor (CIC) capacitor. Figure 1 shows the dramatic increase in capacitance when comparing a planar CIC to our 3D CIC. Both of these devices have equivalent footprint area and dielectric thickness, and thus the increase comes from the higher parallel plate area (capacitance = $A \cdot \epsilon \cdot d^{-1}$, where A is the parallel plate area, ϵ is the permittivity of the dielectric, and d is the width of the dielectric) in our 3D device. The ALD coatings are complete and conformal, as depicted in the SEM micrograph in Figure 2.

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Abstract ID: 863

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Oral Presentation

Topics: Bulk and Gradient Metallic Nanomaterials

Keywords: Nano-tweezers, NiTiCu alloy, Shape-memory, X-ray diffraction

The Effect of Processing on the Structure and Texture of Melt-spun Ti₂NiCu Shape Memory Ribbons

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Melt-spinning is a process that imparts extremely fast solidification of metal alloys into thin ribbons. This often results in an amorphous structure. Further heat treatment transforms the amorphous phase into nanocrystalline. In the current study, melt-spun and heat treated Ti₂NiCu 40 micrometer-thick ribbons were investigated. Depending on the structure and temperature, this smart alloy is capable of demonstrating both outstanding shape memory and super-elasticity. The shape memory property has been used for creating composites (with an elastic deposited layer) to build nano-tweezers that capable of manipulating nano-objects, such as nanotubes and bionanoparticles while heated up to 40-60 °C by laser radiation¹. The shape-memory performance of the Ti₂NiCu ribbon critically depends on the fraction of crystallinity (versus amorphous phase), crystalline structure (needs to be martensitic phase B19 at room temperature), and the phase transformation to austenite (B2) upon heating to the desired temperature, the crystallographic preferred orientation, and the inherent inhomogeneity. All these are a function of the manufacturing process parameters. X-ray diffraction (Malvern-PANalytical Empyrean) was used for the structure determination of the ribbon as a function of the depth below the surface, comparing the air-side with the wheel-side (where the cooling is faster). The tests were repeated to determine the effect of heat treatments that were performed by passing a current through the ribbon. The average crystalline structure (depth about 16 micrometers) of each side was also compared. Lastly, the crystallographic texture of the two sides of the ribbon was studied using pole figures of the B19 and the small residual B2 phase as well. Strong preferred orientation was revealed and the phase transformation relationships were analyzed. The conclusions drawn from the study, combined with our previous performance data will be used to develop excellent shape-memory ribbons through optimal processing. The authors acknowledge the support of the National Science Foundation, award number: CMMI-1626276, MRI for this research.

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Abstract ID: 864**Symposium 1: Functional Biomaterials and Biosensors (FBB)****Oral Presentation**

Topics: Surface properties of biomaterials

Keywords: Carboxymethyl Dextran, FluidFM, RGD, Label-free Biosensor, Cell Micropatterning, Cell Adhesion

Dextran-based hydrogel layers for label-free biosensing and cell micropatterning

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Biofunctional coatings fabricated on transducer surfaces are essential elements of label-free biosensors providing protein- and cell-repellent ability, high immobilization capacity, high conjugability as well as biocompatibility. The carbohydrate dextran can be efficiently used to develop three-dimensional hydrogel layers on biosensor surfaces. Besides the classical bioanalytic applications, such layers enables the spatially controlled chemical modification of the sensor surface for micropatterning with living cells, which has an emerging significance both in the development of cell-on-a-chip or tissue-on-a-chip biosensors and in researching the fundamentals of cell adhesion.

In this work, we present our developed carboxymethyl dextran (CMD)-based hydrogel coatings suitable for cell micropatterning and controlled cell adhesion studies performed by label-free optical biosensors. The CMD layers were covalently grafted to waveguide-type optical biosensor chips and glass slides using EDC/NHS chemistry and chemical crosslinking reaction. The fabricated CMD layers were characterized by contact angle measurements, atomic force microscopy (AFM), spectroscopic ellipsometry as well as x-ray photoelectron spectroscopy (XPS). The protein-repellent ability of the layers were tested by protein adsorption experiments, which were in situ monitored using optical waveguide lightmode spectroscopy (OWLS). The CMD surfaces were conjugated with cell-adhesion inducing cRGDfK (cyclo(Arg-Gly-Asp-D-Phe-Lys)) peptide motifs and its micropatterns were obtained by the novel FluidFM BOT solution. This unique technology combines atomic force microscopy and microfluidics establishing the force-controlled printing of biomolecules directly from liquid phase [1]. Exploiting the original cell-repellent but great conjugation ability as well as hydrogel nature of the CMD layer, we achieved cell micropatterns on the cRGDfK-prints with high contrast to the cell-repellent unmodified CMD background. Owing to the FluidFM printing technology, cell micropatterns with different geometries covering large, cm x cm scale areas could be achieved without using lithography equipment and cleanroom conditions [2].

Key Words: Carboxymethyl Dextran, FluidFM, RGD, Label-free Biosensor, Cell Micropatterning, Cell Adhesion

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Abstract ID: 865

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Plenary

Topics: Realization and application of nanodevices electronics, optoelectronics, photonics, energy harvesting, biological sensing, composite, and so forth

Keywords: Micron/nano materials, Ionization sensor, multi-information detection

The road toward miniaturization and integration of ionization sensors following advanced MEMS

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Micron/nano materials have broad applications for their unique physical and chemical properties. The recent progress in micron/nano materials, especially in carbon nanotubes (CNTs) leads to potential applications on sensing technology. Double-electrode ionization sensors using CNTs has been developed at first, which operated at one order lower voltage than the traditional ionization sensors with millimeter curvature radius electrode, yet they are limited by higher voltage and multi-valued sensitivity. Then triple-electrode ionization sensors were developed, where a tripolar-electrode configuration has been firstly reported, but still showed multi-valued. We proposed a novel triple-electrode ionization sensor, featuring two electric fields with opposite directions, and solved multi-valued problem as well as obtained single-valued sensitivity to gases measured. At the same time, the sensor showed lower power consumption and smaller volume than ever before. In a conclusion, the life span of the ionization sensors using nanomaterials has been prolonged by one order, but is not able to satisfy the applications. Since CNTs are more easily oxidized than metal, gold coating of CNTs was explored, which prolonged the life span of CNTs greatly. At this period, the reports on that the gold nanostructure was prepared by low pressure evaporation method, showed a promising potential of a long life-span ionization sensors, which were verified by one order longer life span than before. Unfortunately, support of the gold nanostructure technique was interrupted, silicon micropillars coated with metal film were explored to replace the gold nanostructure, which exhibited the longest life span, the highest sensitivity, and successfully detected ppt (10⁻¹² L/L) order of ultra-trace gases. Innovatively, the exponential dependence of inter-electrode separation on discharge current enable the ionization sensors identifying different measured parameters with various electrode gaps at the same time, and featuring high integration and miniaturization, which formed a sensor array by the Microelectromechanical Systems (MEMS) fabrication. Artificial intelligence (AI) model based multi-information fusion was explored to get precise values of measured parameters. The sensors showed multi-information detection abilities on gas, haze, temperature, and electromagnetic fields.

Tuesday, 20/Aug/2019 9:00am - 9:45am

Abstract ID: 866 / Keynote-1: 1

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Keynote

Topics: 3D Scaffolds

Keywords: Nano-and Microfabricated Hydrogels

Nano-and Microfabricated Hydrogels for Regenerative Engineering

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Micro- and nanoscale technologies are emerging as powerful tools for controlling the interaction between cells and their surroundings for biological studies, tissue engineering, and cell-based screening. Hydrogel biomaterials have been increasingly used in various tissue engineering applications since they provide cells with a hydrated 3D microenvironment that mimics the native extracellular matrix. We have developed various approaches to merge microscale techniques with hydrogel biomaterials for directing stem cell differentiation and generating complex 3D tissues. In this talk, I will outline our work in controlling the cell-microenvironment interactions by using patterned hydrogels to direct the differentiation of stem cells; including the fabrication and the use of microscale hydrogels for tissue engineering by using a 'bottom-up' and a 'top-down' approach. Top-down approach for fabricating complex engineered tissues involves the use of miniaturization techniques to control cell-cell interactions or to recreate biomimetic microvascular networks within mesoscale hydrogels. Our group has also pioneered bottom-up approaches to generate tissues by the assembly of shape-controlled cell-laden microgels (i.e. tissue building blocks), that resemble functional tissue units. Microgels were fabricated and seeded with different cell types and induced to self-assemble to generate 3D tissue structures with controlled microarchitecture and cell-cell interactions.

Wednesday, 21/Aug/2019 9:00am - 9:50am

Abstract ID: 867 / Plenary: 2

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Plenary

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

Keywords: blue LED

Invention of High Efficient blue LED and Future Solid State Lighting

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Maruska and Tietjen did the first GaN growth by using hydride vapor phase epitaxy in 1969. Since their first GaN growth, a lot of breakthroughs have been achieved for the crystal growth of GaN and InGaN, conductivity control of p-type GaN, and the device structures of LED and laser diodes. Then finally, first high efficient blue LEDs were invented in 1993 [1]. The first white LED was also developed using the blue LED and YAG phosphor by Nichia Chemical Ind., in 1996.

Since first high efficient blue LEDs grown on sapphire were invented in 1993, these blue and white LEDs have been used for all kinds of applications, such as back light of LCD display, general lighting and others. I name these LEDs grown on sapphire and SiC substrate as 1st generation LEDs. These LEDs have been operated at a low current density due to an efficiency droop caused by a high dislocation density and Auger recombination. Recently, high efficient violet LEDs have been developed using GaN substrates by Sora Inc., [2]. It is called GaN on GaN LED. I like to name these high efficient violet LEDs grown on GaN substrates as 2nd generation LEDs because white LEDs made by using the violet LED grown on GaN substrates have superior characteristics in the view of the wavelength stability, efficiency droop, white color quality with a high CRI and the low peak intensity of the blue light which disrupt the circadian cycle.

First violet laser diodes (LDs) were invented in 1995 [3]. Then, those violet LDs have been used for the Blue-Ray DVDs. Now, these blue LDs are used for the application of laser projectors and automobile head lamps with the advantage of the directionality and high light output power density. These laser lighting could be used for a general lighting in the future by reducing the cost and improving the efficiency. I like to name the laser lighting as the 3rd generation solid state lighting.

Tuesday, 20/Aug/2019 9:45am - 10:30am

Abstract ID: 868 / Keynote-1: 2

Symposium 4: Functional Materials for Energy Storage and Conversion Devices (FESC)

Keynote

Topics: Nanogenerators and self-powered nanosystems

Keywords: triboelectric

Maxwell's displacement current governed triboelectric nanogenerator for self-powered systems and blue energy

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Contact electrification (triboelectrification) effect, the most fundamental effect for electricity, has been known for over 2600 years since ancient Greek time, but its scientific mechanism remains unclear. The study of triboelectrification is recently revived due to the invention of the triboelectric nanogenerators (TENGs) by using the coupling of triboelectrification and electrostatic induction effects, which is the most effective approach for converting tiny mechanical energy into electricity for powering small sensors. TENG is playing a vitally important role in the distributed energy and self-powered systems, with applications in internet of things, environmental/infrastructural monitoring, medical science, environmental science and security. In this talk, we first present the physics mechanism of triboelectrification for general materials. Secondly, the fundamental theory of the TENGs is explored based on the Maxwell equations. In the Maxwell's displacement current proposed in 1861, the term $\frac{\partial E}{\partial t}$ gives the birth of electromagnetic wave, which is the foundation of wireless communication, radar and later the information technology. Our study indicates that, owing to the presence of surface polarization charges present on the surfaces of the dielectric media in TENG, an additional term $\frac{\partial P_s}{\partial t}$ should be added in the Maxwell's displacement current, which is the output electric current of the TENG. Therefore, our TENGs are the applications of Maxwell's displacement current in energy and sensors. TENGs have three major application fields: micro/nano-power source, self-powered sensors and blue energy. We will present the applications of the TENGs for harvesting all kind mechanical energy that is available but wasted in our daily life, such as human motion, walking, vibration, mechanical triggering, rotating tire, wind, flowing water and more. Then, we will illustrate the networks based on triboelectric TENGs for harvesting ocean water wave energy, for exploring its possibility as a sustainable large-scale blue energy. Lastly, we will show that TENGs as self-powered sensors for actively detecting the static and dynamic processes arising from mechanical agitation using the voltage and current output signals.

Tuesday, 20/Aug/2019 2:45pm - 3:30pm

Abstract ID: 869 / Keynote-2: 2

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Keynote

Topics: Chemistry of 2D Materials for Energy, Catalysis and Sensing Applications

Keywords: Two-dimensional Structures

Materials Science of Two-dimensional Structures

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Since the discovery of graphene, a large number of materials compositions have been discovered showing stability as two-dimensional structures, with a spectacular range of electronic properties. This talk will focus on the materials science of the emerging field of 2D atomic layers of various compositions. Our work in the past decade ranging from synthesis and characterization to unique property demonstration of these 2D building blocks and their heterostructures will be presented. The concept of nanoscale engineering and the goal of creating new artificially stacked van der Waals solids and 3D constructs will be discussed through a number of examples of 2D structures. The talk will explore the emerging landscape of 2D materials systems that include hybrid compositions and multi-component 2D alloys. Some of the anticipated applications of these materials will be discussed.

Wednesday, 21/Aug/2019 8:10am - 9:00am

Abstract ID: 870 / Plenary: 1

Symposium 5: Functional Low dimensional, Nano and 2D materials (FLNM)

Keynote

Topics: Large Scale Growth & Characterization of 2D-layered oxides, nitrides, carbides and sulfides

Keywords: Transfer technique, 2-dimensional materials, Chemical vapor deposition, Mobility.

Universal Transfer Method for Large Area 2-Dimensional Materials Grown by Chemical Vapor Deposition

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Transfer and integration of nanostructures onto desirable substrates is the prerequisite for their fundamental studies and practical applications. Conventional transfer techniques involving stamping, lift-off and/or striping are greatly limited by the process-specific shortcomings, including the requirement for chemical etchant or high-temperature annealing and the introduction of surface discontinuity and/or contamination that can greatly deteriorate the intrinsic properties of the transferred materials. We have developed a universal transfer method implementable at mild conditions to transfer large area 2-Dimensional (2D) materials grown by chemical vapor deposition method onto various substrates. This technique not only allows the effective transfer to an arbitrary target substrate with a high degree of freedom, but also avoids PMMA etching thereby maintaining the high quality of the transferred 2D materials with minimum contamination. We applied this method to transfer various 2D materials grown on different rigid substrates of general interest, such as graphene on copper foil, h-BN on platinum and MoS₂ on SiO₂/Si. We believe that our method can facilitate the development of nanoelectronics by accelerating the clean transfer and integration of low-dimensional materials into multidimensional structures.