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**AAAFM**

American Association for Advances in  
Functional Materials

**Materials For Life**

**UNIVERSITY OF CALIFORNIA  
LOS ANGELES, USA  
19-22 AUGUST 2019**



# AAAFM

American Association for Advances in  
Functional Materials

Materials For Life

## About AAAFM

World's leading functional materials community, advancing excellence in the materials sciences.

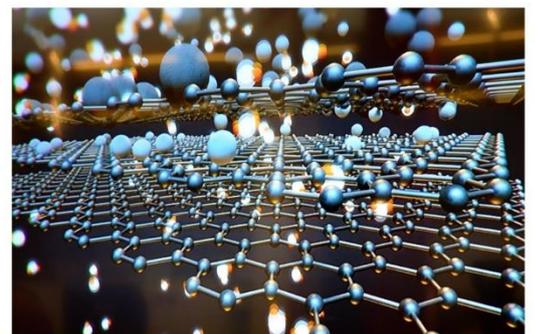
## American Association for Advances in Functional Materials

With foundations rooted in innovation and research, the AAAFM is a globally recognized, functional materials membership society. We are a group of individuals working together for the advancement and benefit of humanity by furthering the focus on functional materials. Being active in this area of study for many years, we have gained members with diverse backgrounds from around the world. Amongst our esteemed members, you will find seasoned professionals at the peak of their careers from fields like education, government and entrepreneurship as well as amateurs who are simply enthusiastic about functional materials.

The purpose of this gathering is to create a platform where people sharing a passion for materials can inspire and guide each other. Since we are a charity, we take measures to use materials in such a way that they can deliver their exceptional potential to benefit the society long-term. Besides enabling enthusiasts to receive professional support from the AAAFM members, we also make a point of connecting with policymakers and the public quite frequently. The main purpose of doing so is to spread awareness about materials and make people understand the potential it holds for the benefit of all humankind.

The core aim of AAAFM Publishing's effort is to transform into a global leader in scientific education and communication. By publishing articles, journals, magazines, online data silos, and e-books, we enable people from around the world to have access to scientific knowledge.

You can also become a part of this advancing movement and help us build the foundation of our discipline's future. You can invest in materials today to see exceptional results tomorrow. By supporting AAAFM's mission to scale up its activities, you will play a proactive role in assisting us to establish a better foundation for future generations.



<https://aaafm.org>

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# AAAFM

American Association for Advances in  
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## American Association for Advances Functional Materials

Shaping a Better Future by Innovating Market Research and Promoting, Supporting, and Accelerating Functional Materials.

AAAFM deals in the following areas:

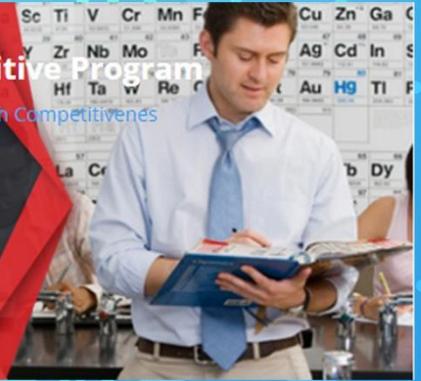
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## Nakamura Award

is a prestigious prize conferred on an outstanding, dynamic researcher for their outstanding achievements and contributions to the field of Functional Materials. The age of the candidates must fall within this age bracket 46-65 years.

### Shuji Nakamura Nobel Prize in Physics 2014



AAAFM honors and recognizes international scientists who have shown, during the course of their professional careers, outstanding achievements in the fields of Functional Materials.

## Award Winners



### Chad A. Mirkin

Mirkin receives the Nakamura Award for his contributions to nanoscale functional materials and the commercial products and process that are based upon them, including the invention and development of spherical nucleic acids and can tilever-free, scanning probe-based, and 3D printing methodologies.



### John A. Rogers

Rogers receives a Nakamura Award for his pioneering contributions to the flexible, stretchable, and wearable electronic systems for health care and exploratory neuroscience.

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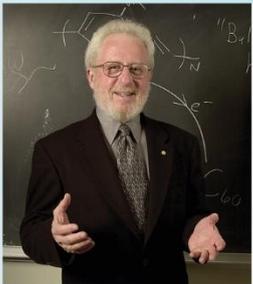
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## Heeger Award

is a prestigious prize conferred on an outstanding, dynamic young researcher for their outstanding achievements and contributions to the field of Functional Materials. The maximum age considered is 45 years.

### Alan J. Heeger Nobel Prize in Chemistry 2000



AAAFM honors and recognizes international scientists who have shown, during the course of their professional careers, outstanding achievements in the fields of Functional Materials.

## Award Winners



### Julia R. Greer

Julia R. Greer receives the Heeger Award for her pioneering research in creating and applying multi-scale 3D architected materials in chemical and biological devices, ultra-light weightenergy storage systems, damage-tolerant fabrics, and additive manufacturing.



### Xiaodong Xu

Xiaodong Xu receives the Heeger Award for his seminal contributions in fundamental understanding the optical, electronic, and quantum properties of novel solid state materials through an elegant integration of nanoscale device design, optical spectroscopy, electrical transport, and scanning photocurrent measurements.

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# AAAFM

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Materials For Life

## International Conference

“Functional Materials for Industrial Revolution”

**August 19-22, 2019.**

### Plenary Speakers



Shuji Nakamura  
University of California,  
Santa Barbara, USA



Ali Khademhosseini  
University of California,  
Los Angeles, USA



Dae Joon Kang  
Sungkyunkwan University,  
Suwon, Korea



Jinlian Hu  
The Hong Kong Polytechnic  
University, Hung Hom,  
Hong Kong



Pulickel Ajayan  
Rice University  
Houston, Texas



Richard B. Kaner  
University of California,  
Los Angeles, California,  
USA



Yunqi Liu  
Institute of Chemistry,  
Chinese Academy of Sciences,  
China



Yury Gogotsi  
Drexel University,  
Philadelphia, USA

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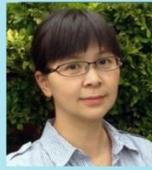
Materials For Life

## International Conference “Functional Materials for Industrial Revolution” August 19-22, 2019.

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University of  
California  
Los Angeles



Yu Huang,  
University of  
California  
Los Angeles



Imran Shakir,  
UCLA,  
KSU. Saudi Arabia

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Sagdicoglu Celep,  
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University of  
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Stavroula Alina  
Kampouri, Ecole  
Polytechnique  
Federal de Lausannes



Tan Sui,  
University  
of Surrey

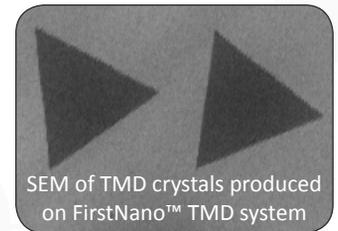
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## FirstNano® EasyTube® TMD MOCVD systems

Flexible Chemistry • Ease of Operation • Safety Focus

Two-dimensional layers of transition metal dichalcogenides (TMDs) such as molybdenum disulfide (MoS<sub>2</sub>) and tungsten diselenide (WSe<sub>2</sub>) exhibit extraordinary optoelectronic properties. Applications for these materials include high speed electronics, flexible devices, next generation solar cells, and touch screen display panels.

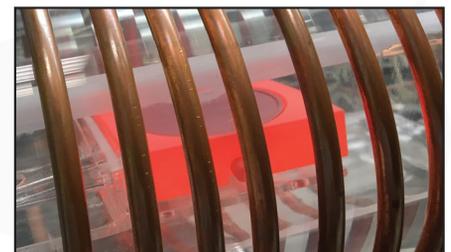


### FirstNano® EasyTube® 3000TMD Single Chamber System

The EasyTube® 3000TMD is designed for wafer-scale growth of uniform 2D TMD layers with abrupt interfaces for the advanced optoelectronics research and development user. The system includes metal organic vapor and hydride gas delivery. Our EasyTube® MOCVD platform is widely used in universities and industry. With >37 years of equipment design and fabrication experience, our company brings a level of know-how that ensures high-performance and usability.

#### Features & Options:

- Horizontal cold-wall reactor
- RF induction heating
- Wafer rotation
- Metal organic vapor delivery for transition metal sources
- Metal organic vapor and/or hydride gas delivery of chalcogen sources
- Flexible source delivery options for dopants/functionalizers/modifiers
- Run and vent manifolds for abrupt interfaces
- Resistance heating up to 1100° C
- Vacuum system
- Safety system
- Our proprietary advanced industrial **CVDWinPrC™** system control and process editing software
- On-site startup assistance
- Optional gas delivery cabinets and panels
- Optional exhaust abatement system
- Many other modules available, contact factory



# TMDC™ Multi Chamber Cluster Tool

The TMDC™ cluster system for wafer scale growth of uniform 2D TMD layers includes a central robotic transfer chamber, up to three (3) process modules, and either a loadlock or glovebox at the load station. Each process module is configured for a particular process and material. By keeping chemistries isolated to each chamber, heterostructures can be synthesized while minimizing risk of cross-contamination. Process modules are independent and can be operated in sequence or in parallel.



## Features & Options:

- Stainless Steel MOCVD growth chamber for single wafer up to 100 mm
  - » System configured with up to three (3) process chambers
  - » Process chambers can be added as a future upgrade
  - » Graphite resistance heating up to 1100° C
  - » Wafer rotation
  - » Metal organic vapor delivery for transition metal sources
  - » Metal organic vapor and / or hydride gas delivery of chalcogen sources
  - » Flexible source delivery options for dopants / functionalizers / modifiers
  - » Run and vent manifolds for abrupt interfaces
  - » Vacuum system
- Central robotic transfer chamber
- Safety system
- Additional process chambers can be configured for different processes
  - » MOCVD
  - » ALD
  - » RTP
  - » Annealing
  - » Other options available, consult factory
- Loading station options:
  - » Open to room
  - » Loadlock
  - » Glovebox
- Our proprietary advanced industrial **CVDWinPrC™** system control and process editing software
- Other modules available, contact factory

We provide turnkey operation by offering gas delivery cabinets and exhaust abatement systems that are integrated with the main system control architecture. For both the EasyTube® 3000TMD and the TMDC, we offer a process development service where we install and run process on your system at our headquarters on Long Island, NY. Advantages of this service include an advanced process training course and expedited process dial-in and time-to-production.

**CVD**  
Equipment  
Corporation

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*WELCOME TO THE CONFERENCE ON AAAFM-  
UCLA 2019*

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## Overview

After the grand success of the 1<sup>st</sup> edition of AAAFM-UCLA Conference, we, the Conference Co-chairs and the organizing committee welcome you again to the 2<sup>nd</sup> International Conference on Functional Materials Technology Key Enabler For Industrial Revolution (AAAFM-UCLA, 2019) that is going to be held at University of California, Los Angeles Campus (UCLA) from August 19-22, 2019 in the sprawling Southern California city and the center of the international film and television industry.

The objective of this international event is to present and share up to date researches and findings in the field of functional materials science. The conference will provide a platform for the researchers to find global partners for future collaboration. More than 900 abstracts have been received from all over the world. A large number of participants including scientists, engineers, educators and students from all over the world will attend this event.

In order to maintain the quality of the presented work, all the abstracts have been reviewed by international researchers carefully. Conference participants will benefit from opportunity to submit full original articles for consideration at Current Applied Physics journal (impact factor 2.01) published by Elsevier.

In addition, the participants of the conference will also be able to attend the talks from our highly-reputed Keynote Speakers from all over the world.

The venue of the conference is always carefully chosen for you to spend quality and enjoyable time on and off the conference. Los Angeles is an ideal location for leisure and recreational activities. Magnificent nature, abundant tourist assets, convenient access and lodgings, warm and friendly people.

We are warm-heartedly extending our welcome to you and hope that you will join us in UCLA for a stimulating Conference, a friendly gathering amongst friends and simply a good time.

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# **SYMPOSIUM 1: Functional Biomaterials and Biosensors (FBB)**

**Wednesday, 21/Aug/2019 6:16pm - 6:28pm**

**Abstract ID: 105**

**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**

**Tan Sui**

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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.

Wednesday, 21/Aug/2019 6:04pm - 6:16pm

**Abstract ID: 113**

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 Behaviour of Nanomedicines

**alexander kros**

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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

References

1. J. Bussmann, S. Sieber, E. van Rooijen, F.L. Bos, H. Zope, J. Shih, L.I. Zone, J. Huwyler, A. Kros,\* and F. Campbell. ACS Nano 12 (2018), 2138-2150.

**Abstract ID: 176**

**Symposium 1: Functional Biomaterials and Biosensors (FBB)**

**Poster Presentation**

*Topics:* Biodetection

*Keywords:* Nanoporous, Monolayer, Carbohydrate, Glycoprotein, Biosensor

### **Recent Applications of Nanoporous Gold to Glycoscience**

**Dharmendra Neupane, Jay Bhattarai, Alexei Demchenko, Keith Stine**

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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.

**Abstract ID: 178**

**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**

**Eun-Hye Jang, Sungwook Chung**

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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 (NH<sub>2</sub>-) 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 NH<sub>2</sub>-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.

Wednesday, 21/Aug/2019 5:28pm - 5:40pm

**Abstract ID: 187**

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**

**Sidika Mine Toker**

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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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Wednesday, 21/Aug/2019 6:40pm - 6:52pm

**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

**Chao Zhong**

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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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**Tuesday, 20/Aug/2019 11:20am - 11:50am**

**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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Wednesday, 21/Aug/2019 5:04pm - 5:16pm

**Abstract ID: 238**

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**

**Yan-Hom Li, Shao-Chun Chen**

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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  $7\text{Hz}$  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.

Wednesday, 21/Aug/2019 4:04pm - 4:16pm

**Abstract ID: 243**

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**

**Yao Yao, Jianfeng Ping, Yibin Ying**

Zhejiang University, China, People's Republic of; [yao\\_yao@zju.edu.cn](mailto:yao_yao@zju.edu.cn)

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 H<sub>2</sub>O<sub>2</sub> 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.

Wednesday, 21/Aug/2019 5:16pm - 5:28pm

**Abstract ID: 252**

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**

**Fengnian Zhao, Jianfeng Ping**

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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.

**Wednesday, 21/Aug/2019 4:16pm - 4:28pm**

**Abstract ID: 264**

**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**

**Noe Alvarez<sup>1</sup>, Peter Miller<sup>1</sup>, Rui Lobo<sup>2</sup>, Vesselin Shanov<sup>1</sup>**

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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 4:04pm - 4:16pm

**Abstract ID: 279**

**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**

**Hye Jin Kim, Hee Ju Ahn, Kyo Seon Hwang**

Department of Clinical Pharmacology and Therapeutics, Kyung Hee University, Korea, Republic of (South Korea); [hvejinkim.mail@gmail.com](mailto:hvejinkim.mail@gmail.com)

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  $1.52 \pm 0.03$  and  $0.90 \pm 0.03$  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: 294**

**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**

**SHREOSI CHATTERJEE, SURAJIT DAS**

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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 compounds<sup>1</sup>. 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 Fe<sup>3+</sup> and Fe<sup>2+</sup> 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<sup>-1</sup> and 1635 cm<sup>-1</sup>, 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<sup>-1</sup> 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.

Wednesday, 21/Aug/2019 5:16pm - 5:28pm

**Abstract ID: 324**

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

**Geeta Bhatt, Shantanu Bhattacharya**

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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.

Wednesday, 21/Aug/2019 4:40pm - 4:52pm

**Abstract ID: 326**

**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 Almicci<sup>1,2</sup>, Susanna Martín-Vañó<sup>3,4</sup>, Joan Montero<sup>1</sup>, David Caballero<sup>5,6</sup>, Rosa Noguera<sup>3,4</sup>, Josep Samitier<sup>1,2,3</sup>**

<sup>1</sup>Institute for Bioengineering of Catalonia, Spain; <sup>2</sup>Department of Electronics and Biomedical Engineering, University of Barcelona, Spain; <sup>3</sup>Networking Biomedical Research Center (CIBER), Madrid, Spain; <sup>4</sup>Dpt Pathology, Medical School, University of Valencia (DP-UV)/INCLIVA, Spain; <sup>5</sup>3B's Research Group - Biomaterials, Biodegradables and Biomimetics, University of Minho, Headquarters of the European Institute of Excellence on Tissue Engineering and Regenerative Medicine, AvePark - Parque da Ciência e Tecnologia, 4805-017 Barco, Guimarães, Portugal; <sup>6</sup>ICVS/3B's - PT Government Associate Laboratory, Braga/Guimarães, Portugal; [ealmici@ibecbarcelona.eu](mailto:ealmici@ibecbarcelona.eu)

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 nanofabrication 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: 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**

**Marioara Moldovan<sup>1</sup>, Marcela Rosu<sup>2</sup>, Cristina Prejmerean<sup>1</sup>, Doina Pordan<sup>1</sup>, Violeta Popescu<sup>3</sup>, Codruta Sarosi<sup>1</sup>, Rahela Carpa<sup>4</sup>**

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<sup>2</sup>National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania; <sup>3</sup>Physics and Chemistry Department, Technical University of Cluj-Napoca, Romania;

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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 SiO<sub>2</sub>, and ZrO<sub>2</sub> respectively. Five experimental biomaterials were made using the BisGMA organic matrix (synthesized in our laboratory)/TEGDMA(Aldrich) and inorganic phase: (HA-SiO<sub>2</sub>, barium glass, GO-SiO<sub>2</sub>: 1%, 0,8% - for GS1, GS2: and HA-Zr, barium glass, GO-ZrO<sub>2</sub>:1%, 0,8% for GZ1, GZ2) and GC (HA-Zr, HA-SiO<sub>2</sub>, 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-SiO<sub>2</sub> graphene

**Abstract ID: 338**

**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**

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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 cm<sup>2</sup> 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 image 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.

Wednesday, 21/Aug/2019 5:28pm - 5:40pm

**Abstract ID: 353**

**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**

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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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Wednesday, 21/Aug/2019 6:40pm - 6:52pm

**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**

**Charles Patrick Collier<sup>1</sup>, Joseph Najem<sup>1</sup>, Graham Taylor<sup>1</sup>, Ryan Weiss<sup>2</sup>, Md. Sakib Hasan<sup>2</sup>, Garrett Rose<sup>2</sup>, Catherine Schuman<sup>1</sup>, Alex Belianinov<sup>1</sup>, Stephen Andy Sarles<sup>2</sup>**

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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.

Wednesday, 21/Aug/2019 4:16pm - 4:28pm

**Abstract ID: 434**

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**

**Wenting Qiu<sup>1</sup>, Zhangdi Lu<sup>1</sup>, Yanxiu Li<sup>2</sup>, Yuan Xiong<sup>2</sup>, Andrey L. Rogach<sup>2</sup>, Stefan Nagl<sup>1</sup>**

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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 CsPbBr<sub>3</sub> quantum dots (CsPbBr<sub>3</sub>-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

Wednesday, 21/Aug/2019 4:28pm - 4:40pm

**Abstract ID: 464**

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**

**Andrey Turchanin**

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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 (NH<sub>2</sub>-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 NH<sub>2</sub>-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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Wednesday, 21/Aug/2019 5:52pm - 6:04pm

**Abstract ID: 474**

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**

**Sadagopan Krishnan, Charuksha Walgama, Vini Singh, Gayan Premaratne, Rajasekhara Nerimetla, Jinesh Niroula**

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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: 478**

**Symposium 1: Functional Biomaterials and Biosensors (FBB)**

**Poster Presentation**

*Topics:* Advances in Enzymatic and Non-Enzymatic Biosensors

*Keywords:* Electrochemical aptasensor; Magnetic biocomposites; Pb<sup>2+</sup>-dependent DNAzyme; Thrombin

**A Label-Free Electrochemical Aptasensor Based On Magnetic Biocomposites with Pb<sup>2+</sup>-Dependent DNAzyme for the Detection of Thrombin**

**Chunhong Zhu, Wanying Zhu, xuemin zhou**

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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 Pb<sup>2+</sup>-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 Pb<sup>2+</sup>-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.

Wednesday, 21/Aug/2019 3:52pm - 4:04pm

**Abstract ID: 497**

**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 (PBF1), which uses a diaz-18-crown-6 as a ligand and a benzofuran derivative as the fluorophore. Unfortunately PBF1, 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 colocalization 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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Wednesday, 21/Aug/2019 5:40pm - 5:52pm

**Abstract ID: 507**

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**

**Lan Li<sup>1</sup>, Jiayi Li<sup>2</sup>, Jiamin Guo<sup>3</sup>, Huikang Zhang<sup>2</sup>, Xin Zhang<sup>1</sup>, Caiyun Yin<sup>1</sup>, Liming Wang<sup>2</sup>, Yishen Zhu<sup>1</sup>, Qingqiang Yao<sup>2</sup>**

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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 3:40pm - 3:52pm

**Abstract ID: 540**

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**

**Elena Yunda<sup>1,2</sup>, Fabienne Quilès<sup>2</sup>, David Horwat<sup>1</sup>, Halima Alem<sup>1</sup>**

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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 (-CH<sub>3</sub>) and positively charged (-NH<sub>2</sub>) 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: 561**

**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**

**Albena Daskalova<sup>1</sup>, Irina Bliznakova<sup>1</sup>, Anton Trifonov<sup>2</sup>, Liliya Angelova<sup>1</sup>, Heidi Declercq<sup>3</sup>, Ivan Buchvarov<sup>2</sup>**

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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 (ZrO<sub>2</sub>) insertion will contribute to achieving enhanced mechanical properties of the interface layer. We synthesize thin chitosan (CH) /Hydroxyapatite (HAp)/ ZrO<sub>2</sub> 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.

Wednesday, 21/Aug/2019 3:52pm - 4:04pm

**Abstract ID: 576**

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 constructed 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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Wednesday, 21/Aug/2019 4:52pm - 5:04pm

**Abstract ID: 585**

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: 591**

**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  $\mu$ M. At the optimized conditions with 2.0 mM crosslinkers and 300 $\mu$ 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.

Wednesday, 21/Aug/2019 6:04pm - 6:16pm

**Abstract ID: 629**

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**

**El-Said Ibrahim El-Shafey, Haider Al lawati, Saleh Al-Busafi, Syeda nahed furqan Ali**  
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Acidic dehydrated carbon (DC) was prepared from date palm leaflets via sulfuric acid dehydration at 200 oC. 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, pHzpc, 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 (chlorphniramine, 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 m<sup>2</sup>/g shows better adsorption properties of methylene blue than AC (1056 m<sup>2</sup>/g). Dominant forces of adsorption varied from carbon to another. Thermodynamic parameters showed that the adsorption processes are spontaneous and endothermic with  $\Delta H$  falling within physical adsorption processes. column studies showed better performance on functionalized carbons than activated carbon.

**Abstract ID: 637**

**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**

**Jing Wang<sup>1</sup>, Bei Zhang<sup>2</sup>, Yong Ren<sup>1</sup>**

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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  $1 \times 10^{-7}$  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: 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.

Wednesday, 21/Aug/2019 4:40pm - 4:52pm

**Abstract ID: 658**

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**

**Hamdy Youssef, Najat Alghamdi**

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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: 669**

**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.<sup>1</sup> 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.<sup>2-3</sup> 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-diatyrylanthracene (DSA) derivate unit, a typical AIE fluorogen,<sup>4</sup> 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: 697**

**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 5:04pm - 5:16pm

**Abstract ID: 698**

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: 760**

**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**

**Shili Xiao<sup>1,2</sup>, Qingyan Peng<sup>2</sup>, Yongzhen Tao<sup>1</sup>, Xiangyang Shi<sup>3</sup>, Weilin Xu<sup>1</sup>**

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Electrospun nanofibrous scaffold is promising in tissue engineering due to its 2D and 3D fibrous structure which is analogous 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 permeability<sup>1</sup>. Furthermore, these nanofibrous scaffolds can be “activated” by loading biochemical signals (e.g. proteins, genes) which will help to direct cell behavior<sup>2</sup>. Herein, we developed pDNA (encoding Enhanced Green Fluorescent Protein (EGFP))-activated nanofibrous scaffolds by chemical grafting the fifth generation amino-terminated polyamidoamine (G5.NH<sub>2</sub>) 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.NH<sub>2</sub>-modified PLGA nanofibrous mats, indicating the successful grafting of G5. NH<sub>2</sub> on the nanofibers. Meanwhile, the surface roughness of PLGA nanofiber was greatly increased after grafting G5.NH<sub>2</sub> 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.NH<sub>2</sub>-grafted PLGA nanofibers and (b) NIH 3T3 cells on G5.NH<sub>2</sub>-grafted PLGA nanofibers, (c) Fluorescence microscopy image showing EGFP expression on G5.NH<sub>2</sub>-grafted PLGA nanofibers 48 h post-transfection.

Wednesday, 21/Aug/2019 6:28pm - 6:40pm

**Abstract ID: 771**

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 to 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  $\mu\text{m}$  in size. The cut-off size was reduced by 26.4 % from 2.5  $\mu\text{m}$  to 1.84  $\mu\text{m}$  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: 782**

**Symposium 1: Functional Biomaterials and Biosensors (FBB)**

**Poster Presentation**

*Topics:* Anti-cancer therapy

*Keywords:* Nanostructures, B<sub>4</sub>C, 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 (<sup>10</sup>B 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 (B<sub>4</sub>C). 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 B<sub>4</sub>C 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, B<sub>4</sub>C can be a promising direct boron compound for the treatment of malignant tumors using BNCT.

**Abstract ID: 783**

**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**

**Yaşar Murat Elçin<sup>1,2</sup>, Mahmut Parmaksiz<sup>2</sup>, Murat Taner Vurat<sup>1,2</sup>, Özge Lalegül-Ülker<sup>2</sup>, Serap Durkut<sup>2</sup>, Aysel Koç-Demir<sup>2</sup>, Ayşe Eser Elçin<sup>2</sup>**

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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).

Wednesday, 21/Aug/2019 4:52pm - 5:04pm

**Abstract ID: 790**

**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**

**Omar Uribe<sup>1</sup>, R. Godinez<sup>1</sup>, J. Morales<sup>2</sup>, Myrian Velasco<sup>3</sup>, R. Olayo<sup>2</sup>**

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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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Wednesday, 21/Aug/2019 4:28pm - 4:40pm

**Abstract ID: 792**

**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  $\mu\text{M}$  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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Wednesday, 21/Aug/2019 5:52pm - 6:04pm

**Abstract ID: 822**

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**

**Tarakdas Basu, Sanchita Nandy**

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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 antibacterial 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  $\text{AgNO}_3$ , using hydrazine hydrate as the reducing agent and gelatin and poly-vinyl pyrrolidone (PVP) as the capping agents. The particles are core-shell in structure with  $\text{Cu}_0$  core and  $\text{Ag}_0$  shell, about  $(100 \pm 10)$  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. flexneri2a, 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.

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Wednesday, 21/Aug/2019 5:40pm - 5:52pm

**Abstract ID: 838**

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**

**Yitayal Admassu Workie<sup>1</sup>, Toyoko Imae<sup>1</sup>, Marie Pierre Krafft<sup>2</sup>**

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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 NO<sub>2</sub> 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

Wednesday, 21/Aug/2019 3:40pm - 3:52pm

**Abstract ID: 844**

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

**Golbarg MohammadiRoozbahani<sup>1</sup>, Xiaohan Chen<sup>1</sup>, Youwen Zhang<sup>1</sup>, Mona H Soflaee<sup>2</sup>, Xiyun Guan<sup>1</sup>**

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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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Wednesday, 21/Aug/2019 6:16pm - 6:28pm

**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

**Andras Saftics<sup>1</sup>, Barbara Türk<sup>1</sup>, Tamás Gerecsei<sup>1</sup>, Attila Sulyok<sup>2</sup>, Norbert Nagy<sup>3</sup>, Inna Szekacs<sup>1</sup>, Sándor Kurunczi<sup>1</sup>, Robert Horvath<sup>1</sup>**

<sup>1</sup>Nanobiosensorics Laboratory, EK MTA, Hungary; <sup>2</sup>Thin Film Physics Department, EK MTA, Hungary; <sup>3</sup>Photonics Department, EK MTA, Hungary; [saftics.andras@energia.mta.hu](mailto:saftics.andras@energia.mta.hu)

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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**Tuesday, 20/Aug/2019 8:30am - 9:00am**

**Abstract ID: 866**

**Symposium 1: Functional Biomaterials and Biosensors (FBB)**

**Keynote**

*Topics:* 3D Scaffolds

*Keywords:* Nano-and Microfabricated Hydrogels

### **Nano-and Microfabricated Hydrogels for Regenerative Engineering**

**Ali Khademhosseini**

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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 6:28pm - 6:40pm

**Abstract ID: 888**

Symposium 1: Functional Biomaterials and Biosensors (FBB)

Poster Presentation

Topics: Drug delivery/controlled release

Keywords: Microsphere, Gallic Acid, Controlled Release, Polyphenols, Cancer

### **Antioxidant and Anticancer Activities of Gallic Acid Loaded Sodium Alginate Microspheres**

**Aslihan Demirkaya<sup>1</sup>, Ebru Kondolot Solak<sup>2</sup>, Advive Gulcin Sagdicoglu Celep<sup>3</sup>**

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Antioxidant and Anticancer Activities of Gallic Acid Loaded Sodium Alginate Microspheres

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Polyphenols are compounds that contain more than one phenol group per molecule and are found in several foods such as vegetables, fruits, legumes and tea. They are of great interest due to their beneficial effects against many diseases such as, cardiovascular diseases, neurodegenerative diseases and cancer. Polyphenols are of great importance for health due to their high antioxidant properties. Gallic acid (GA) (3,4,5-trihydroxyl-benzoic acid), a member of the tannins group of polyphenols, is a powerful antioxidant. Cytotoxic effects of GA on various cancer cells have been proven with several studies. GA has many beneficial effects such as wound healing, antiviral, antifungal, antibacterial and antimutagenic effects. Microspheres are carriers varying in size from 1-1000  $\mu\text{m}$ , where the active substance is trapped in the polymer matrix. A controlled release profile is aimed at the target region by preserving the loss of substance and activity until the active substance reaches the target region. In this study, GA containing microspheres were formed with NaAlg which is a natural polymer in formulations with GA / NaAlg ratio of 1 / 1-1 / 8 by using water / oil / water emulsion method, and CaCl<sub>2</sub> was used as a crosslinker. The microsphere yields of the obtained microspheres were 15.55-80.27%; arrest efficiencies ranged from 11.26 to 72.64%. Release studies of microspheres were performed at pH 7.4. Optimum microsphere forming conditions were determined as GA / NaAlg ratio 1/8 and crosslinking time 30 min. The microspheres formed were found to arrest GA and exhibit a controlled release profile. Microspheres were characterized by SEM, DSC, XRD, FTIR analysis. It was demonstrated by DPPH method that GA retained antioxidant activity in microspheres and that retain anticancer activity by using MTT analysis on Caco-2 cells. It is important to carry out necessary studies on GA-loaded NaAlg microspheres which have high potential to be used in adjunct and complementary therapies.

**Wednesday, 21/Aug/2019 8:10am - 8:40am**

**Abstract ID: 891**

**Symposium 1: Functional Biomaterials and Biosensors (FBB)**

**Keynote**

*Topics:* Intelligent biomaterials

*Keywords:* Biocompatible Optoelectronic Systems

### **Soft, Biocompatible Optoelectronic Systems as Neural Interfaces**

**John A. Rogers**

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Advanced optoelectronic devices that are capable of intimate integration with the brain and the peripheral nervous system have the potential to accelerate progress in neuroscience research and to spawn new therapies for neurological disorders. Specifically, capabilities for injecting electronics, light sources, photodetectors, multiplexed sensors, programmable microfluidic networks and other components into precise locations of the deep brain and for softly laminating them onto targeted regions of the surfaces of the brain or the peripheral nerves will open up unique and important opportunities in stimulation, inhibition and real-time monitoring of neural circuits. In this talk, we will describe foundational concepts in materials science and assembly processes for these types of technologies, in 1D, 2D and 3D architectures. Examples in system level demonstrations include experiments on freely moving animals with ‘cellular-scale’, injectable probes for optogenetics research, with 3D mesoscale networks for study of neural signal propagation, and with closed-loop systems for control of bladder function.

## **SYMPOSIUM 2: Functional Composite Materials (FCM)**

Wednesday, 21/Aug/2019 2:00pm - 2:12pm

**Abstract ID: 118**

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

**Justyna Kozłowska, Weronika Prus, Natalia Stachowiak**

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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

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**Abstract ID: 131**

**Symposium 2: Functional Composite Materials (FCM)**

**Poster Presentation**

*Topics:* Ceramic based composites

*Keywords:* CeO<sub>2</sub>, Heterojunction, Sensor

**Growth of Nickel Oxide on CeO<sub>2</sub> Nanoparticles Obtained In Different Morphologies Applied As Gas Sensor**

**Rafael APARECIDO CIOLA AMORESÍ<sup>1</sup>, Regiane C Oliveira<sup>2</sup>, Priscila B Almeida<sup>2</sup>, Maria A Zaghete<sup>3</sup>, Julio Sambrano<sup>4</sup>, Miguel Ponce<sup>5</sup>, Elson Longo<sup>2</sup>, Alexandre Z Simões<sup>1</sup>**  
<sup>1</sup>UNESP, Brazil; <sup>2</sup>UFSCar, Brazil; <sup>3</sup>UNESP, Chemical Institute-Ara, Brazil; <sup>4</sup>UNESP, Bauru, Brazil; <sup>5</sup>University of Mar del Plata (UNMdP), Argentina; [rafaelciola@yahoo.com.br](mailto:rafaelciola@yahoo.com.br)

Particles of CeO<sub>2</sub> 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 CeO<sub>2</sub> nanoparticles were examined as a function of time and catalytic agent concentration used in the microwave assisted hydrothermal synthesis method. We obtained particles of CeO<sub>2</sub> 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 CeO<sub>2</sub> preferential surfaces with Ni<sub>2</sub>O<sub>3</sub>, forming the heterojunction with respect to the CO gas sensing application.

**Abstract ID: 132**

**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**

**Prasad G. Mahajan<sup>1</sup>, Nilam C. Dige<sup>2</sup>, Balasaheb D. Vanjare<sup>1</sup>, Ki Hwan Lee<sup>1</sup>**

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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-Dimethylantracene (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.

**Wednesday, 21/Aug/2019 4:40pm - 4:52pm**

**Abstract ID: 142**

**Symposium 2: Functional Composite Materials (FCM)**

**Oral Presentation**

*Topics:* Ceramic based composites

*Keywords:* Graphene, Polymer Derived Ceramic, Composites

### **Polymer Derived Ceramic Composites with Graphene**

**Lei Zhai**

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Polymer derived ceramics (PDCs) include a class of ceramics (e.g. SiC, SiCO, SiCN, BCN, BN, Si<sub>3</sub>N<sub>4</sub>, and etc.) synthesized by a thermal decomposition of polymeric precursors. PDCs have unique nanostructures that grant various attractive properties such as low density (~2g/cm<sup>3</sup>), 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: 145**

**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,  $\text{EuSr}_2\text{Ca}_2\text{Cu}_2\text{O}_{6.5}$  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  $\text{EuSr}_2\text{Ca}_2\text{Cu}_2\text{O}_{6.5}$  has a promising potential for metamaterial coating applications.

Wednesday, 21/Aug/2019 5:28pm - 5:40pm

**Abstract ID: 147**

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Polymeric composites

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

### **Epoxy/WO<sub>3</sub> Nano Composites as an Eco-Friendly Gamma Ray Shielding Materials**

**Isa Emin Ongun<sup>1</sup>, Yaşar Karabul<sup>1</sup>, Mustafa Çağlar<sup>2</sup>, Mehmet Kılıç<sup>1</sup>, Zeynep Güven Ozdemir<sup>1</sup>, Orhan İçelli<sup>1</sup>**

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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/WO<sub>3</sub> nano composites were prepared with different WO<sub>3</sub> nano particle weights percentages varying from 5 to 20. The WO<sub>3</sub> 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 WO<sub>3</sub> nano particles in the epoxy matrix was also viewed by Scanning Electron Microscope (SEM). The influence of WO<sub>3</sub> 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.

**Wednesday, 21/Aug/2019 2:00pm - 2:12pm**

**Abstract ID: 157**

**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**

**Yongmei Zheng**

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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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Wednesday, 21/Aug/2019 4:52pm - 5:04pm

**Abstract ID: 190**

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: 195**

**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**

**Matheus Couto Crisóstomo, Joaquim Carlos Gonçalez, Claudio Henrique Soares Del Menezzi**

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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 Gonçalez (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.

Tuesday, 20/Aug/2019 3:24pm - 3:36pm

**Abstract ID: 201**

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**

**Mulat Alubel ABTEW<sup>1,2,3,4</sup>, François BOUSSU<sup>2,3</sup>, Pascal BRUNIAUX<sup>2,3</sup>, Carmen LOGHIN<sup>1</sup>, Irina CRISTIAN<sup>1</sup>, Yan CHEN<sup>4</sup>, Lichuan WANG<sup>4</sup>**

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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

Wednesday, 21/Aug/2019 2:36pm - 2:48pm

**Abstract ID: 216**

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

*Topics:* Composites in Innovative Applications

*Keywords:* Lost circulation, Lost circulation materials, Shape memory polymer, Composite, Thermal-response and intelligent materials

### **Preparation and Study on Thermal-Response and Intelligent Composite Lost Circulation Material Based On Shape Memory Polymer in Drilling Engineering**

**Dan Bao<sup>1</sup>, Zhengsong Qiu<sup>1</sup>, Haiyi Zhong<sup>1</sup>, Xin Zhao<sup>1</sup>, Ganghua Chen<sup>2</sup>**

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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. Lost circulation materials have been widely used to stop or mitigate losses. 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. In most of the cases, the size of the loss zone is not known, making conventional lost circulation materials (LCMs) difficult to plug the loss zone. In this study, a novel thermal-response and intelligent LCM was prepared. It is a thermal-response shape memory polymer. The molecular structure was analyzed by the Fourier transform infrared spectroscopy (FT-IR). The glass transition temperature ( $T_g$ ) was tested by Different scanning calorimetry (DSC). The shape memory properties were evaluated by a bend-recovery test instrument. The expansion and mechanical properties of particles were investigated under high-temperature and high-pressure. Fracture sealing testing apparatus was used to evaluate sealing performance. Research results indicated that the  $T_g$  of the TI-LCM was 70°C. The shape fixation ratio was more than 99% at room temperature, and the shape recovery ratio was 100% above the  $T_g$ . The particle was flaky before activation. It expanded to granular shape and the thickness increased when activated. The activated TI-LCM particles had high crush strength. The expansion of the TI-LCM particles could self-adaptively bridge and seal the fracture without knowing the width. The addition of TI-LCM particles could seal the tapered slot with the entrance width of 2mm, 3mm and 4mm without changing the LCM formulation. The prepared TI-LCM could cure fluids loss in fractured formation efficiently. This study offers a promising route to cure the severe loss in fractured formations.

Wednesday, 21/Aug/2019 1:00pm - 1:12pm

**Abstract ID: 217**

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**

**Ming-Hwa R. Jen, Guan-Ting Guo, Ying-Hui Wu, Ying-Jing Chen**

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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 SiO<sub>2</sub> of optimal 1 wt.%.

The geometry and dimensions of specimens were  $L \times W \times t = 210 \times 25 \times 1.55$  mm<sup>3</sup>. 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 6:16pm - 6:28pm

**Abstract ID: 218**

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**

**Manasa G<sup>1</sup>, Ronald Jerald Mascarenhas<sup>1</sup>, Ashis K Satpati<sup>2</sup>, Basavanakote M Basavaraja<sup>3</sup>, Sriram Kumar<sup>2</sup>**

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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  $\mu$ M. 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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Wednesday, 21/Aug/2019 5:04pm - 5:16pm

**Abstract ID: 228**

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 Chen<sup>1</sup>, Yifan Li<sup>2</sup>, Eric Meshot<sup>1</sup>, Ngoc Bui<sup>1</sup>, Rong Zhu<sup>2</sup>, Myles Herbert<sup>2</sup>, Sei Jin Park<sup>1</sup>, Steven Buchsbaum<sup>1</sup>, Melinda Jue<sup>1</sup>, Kuang Jen Wu<sup>1</sup>, Timothy M. Swager<sup>2</sup>,  
**Francesco Fornasiero<sup>1</sup>**

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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/m<sup>2</sup>day, 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.<sup>1</sup>

When actuating polymers responsive to G-agents are grafted to the CNT membrane surface,<sup>2,3</sup> these multifunctional membranes are able to switch from a breathable state with MVTR > 4,000 gr/m<sup>2</sup>day to a protective state with MVTR > 1,000 gr/m<sup>2</sup>day 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.

**Abstract ID: 248**

**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**

**Zhaoxia GUO, Hansong LI, Qiyang ZHANG, Boyuan ZHANG, Jian YU**

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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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Wednesday, 21/Aug/2019 2:48pm - 3:00pm

**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

**Wednesday, 21/Aug/2019 3:00pm - 3:12pm**

**Abstract ID: 250**

**Symposium 2: Functional Composite Materials (FCM)**

**Oral Presentation**

*Topics:* Design and application of composite structures

*Keywords:* hybrid surface, hydrophobic-hydrophilic surface, dehumidification, condensation

**Development of nano-structured hybrid hydrophobic-hydrophilic surface to improve condensation heat transfer**

**Mahmood Yaghoubi, M. Hormozi, S Fosehat**

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Surface wettability plays a significant role on efficiency of condensation heat transfers such as in water desalination and dehumidification of humid air. It is well known that application of a hybrid hydrophobic-hydrophilic surface will improve condensation performance and increase dehumidification. Despite many efforts, there is lack of a reliable, straightforward and suitable industrial method to achieve an appropriate hybrid surfaces mainly to produce fresh water from humid air. In this study attempt is made to achieve a new hybrid surface with application of Anodizing and Electrophoretic Deposition, which showed particular properties of a hydrophobic-hydrophilic hybrid surface. For making this dehumidification surface, initially we used phosphoric acid as the anodizing electrolyte to reach over 200 nm structured holes on a commercial aluminum substrate. Next functionalized silica nanoparticles were inserted into the prepared holes by electrophoretic deposition method. Due to the semi-conductor feature of the anodized aluminum oxide thin layer, the deposition occurred only with a limited parameters. The silica particles with hydrophobic property alongside aluminum oxide with hydrophilic nature provided a hybrid feature to the prepared surface. The constructed surface is tested to condense water from humid air, it was found that the fabrication method showed an exceptional characteristic in condensation heat transfer enhancement and can be used widely for industrial applications.

**Tuesday, 20/Aug/2019 1:24pm - 1:36pm**

**Abstract ID: 256**

**Symposium 2: Functional Composite Materials (FCM)**

**Oral Presentation**

*Topics:* Metal matrix composites

*Keywords:* Multifiber Composite, Copper, Functional Properties

### **Cu-Bi multifiber composite wire**

**Wojciech Gluchowski, Zbigniew Rdzawski, Marcin Maleta, Justyna Domagała-Dubiel**

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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.

Wednesday, 21/Aug/2019 5:16pm - 5:28pm

**Abstract ID: 265**

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

**Yufan Zhang, Zhong Li, Xin Zhou**

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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  $2280 \text{ m}^2 \cdot \text{g}^{-1}$  with a pore volume of  $0.69 \text{ cm}^3 \cdot \text{g}^{-1}$ . More importantly, UiO-67-bpy showed a preferential adsorption of propane over propylene with propane capacity of  $9.70 \text{ mmol} \cdot \text{g}^{-1}$  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.

Tuesday, 20/Aug/2019 2:36pm - 2:48pm

**Abstract ID: 274**

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**

**Ngoc A. Nguyen, Christopher C. Bowland, Jong K. Keum, Lilin He, Amit K. Naskar**

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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: 295**

**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**

**Hyeon-Gyun Im, Hoy Yul Park, Dong Jun Kang**

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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: 298**

**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**

**Dong Jun Kang, Hyo Yul Park, Hyeon-Gyun Im**

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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.

**Tuesday, 20/Aug/2019 2:00pm - 2:12pm**

**Abstract ID: 299**

**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)**

**Vikas Vinayak Chaudhari, Swadesh Sandesh Dixit**

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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: 303**

**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**

**Wooteck Kwon, Su-Bin Ahn, Yoonjoo Lee, Younghee Kim, Jung Hyun Kim**

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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.

Wednesday, 21/Aug/2019 1:48pm - 2:00pm

**Abstract ID: 319**

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 MoS<sub>2</sub>-Upconversion Nanoparticles Nanocomposite**

**Sandip Ghosh, Wen Cheng Chiang, Surojit Chattopadhyay**

National Yang-Ming University, Taiwan; [ghosh.sandip36@gmail.com](mailto:ghosh.sandip36@gmail.com)

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 MoS<sub>2</sub> 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<sup>-1</sup> is obtained for 980 nm at 1 V bias and a lowest responsivity of 81 A W<sup>-1</sup> is obtained of 808 nm at 0.1V bias. The broadband nature of photoabsorption was attributed to the few layer MoS<sub>2</sub>, 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.

References:

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2. J.-Y. Wu, Y.T. Chun, S. Li, T. Zhang, J. Wang, P.K. Shrestha, D. Chu, Advanced Materials 30 (2018), 1705880.

**Abstract ID: 321**

**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**

**Sang Heon LEE**

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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 3:52pm - 4:04pm

**Abstract ID: 322**

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Shape-memory alloy

Keywords: Ferromagnetic Shape Memory Alloys, Multifunctional alloys, NiMnGa

### **Microstructure, Magnetic Behaviour and Nanomechanical Characterization of NiMnGa-Based Multifunctional Ferromagnetic Shape Memory Alloys**

**Amadeusz Łaszcz, Mariusz Hasiak, Jerzy Kaleta**

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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 Ni<sub>50</sub>Mn<sub>25</sub>Ga<sub>20</sub>X<sub>5</sub> (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 Ni<sub>50</sub>Mn<sub>25</sub>Ga<sub>20</sub>Gd<sub>5</sub> 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 Ni<sub>50</sub>Mn<sub>25</sub>Ga<sub>20</sub>Ti<sub>5</sub> alloy and each individual phase of the dual-phase Ni<sub>50</sub>Mn<sub>25</sub>Ga<sub>20</sub>Gd<sub>5</sub> 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.

References

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Wednesday, 21/Aug/2019 1:00pm - 1:12pm

**Abstract ID: 336**

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**

**Jaroslav Kaluzny<sup>1</sup>, Krzysztof Kempa<sup>5</sup>, Andrzej Kulczycki<sup>4</sup>, Tomasz Runka<sup>2</sup>, Marek Nowicki<sup>2</sup>, Adam Piasecki<sup>3</sup>, Bartosz Gapinski<sup>3</sup>, Grzegorz Kinal<sup>1</sup>, Aleksander Stepanenko<sup>1</sup>, Dawid Gallas<sup>1</sup>, Jerzy Merkisz<sup>1</sup>**

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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.

[1] J. Kałużny, A. Merkisz-Guranowska, M. Giersig, K. Kempa, International Journal of Automotive Technology, Vol. 18, No. 6, pp. 1047–1059 (2017)

**Abstract ID: 343**

**Symposium 2: Functional Composite Materials (FCM)**

**Poster Presentation**

*Topics:* Polymeric composites

*Keywords:* Responsive fabric, Micro-climate, Body heat, Metabolism.

**Mechanically strong, shape memory polyurethane membrane for thermo-regulating textile**

**Md Anwar Jahid, Jinlian Hu**

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The human body releases heat via four mechanisms: conduction, convection, evaporation, and radiation. The normal core temperature of the human body is around 37°C, metabolism may be negatively affected and enzymes/proteins destroyed if the core temperature rises above 45°C. To prevent such overheating, we developed an Evaporative-Radiative-Convective Fabric (ERCF) which can control the personal microclimate of the human body through a cooling mechanism (evaporation of perspiration, air convection and emission of heat radiation directly into the environment). In this work, we fabricated the thermo-moisture sensitive polyurethane/silica aerogel composite membrane which showed super evaporative and radiative effects and which can facilitate the convection process of the human body. We also fabricated the sensitive membrane-based textile which can cool down the human body by releasing body heat. The developed material possessed robust mechanical properties for the longevity of the material, high water evaporative ability and air permeability to provide comfort to the wearer. Microclimate controlled clothing can release approximately 85% of body heat.

Wednesday, 21/Aug/2019 5:40pm - 5:52pm

**Abstract ID: 347**

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

*Topics:* Design and application of composite structures

*Keywords:* Radiative Coating, Buildings, Passive Cooling, Thermal comfort, Energy savings

### **Development of A New Radiative Coating For Buildings To Achieve Passive Cooling And Energy Saving**

**Jianheng CHEN, Lin Lu, Hong Zhong, Yaxiong Ji**

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A new radiative coating based on hollow glass microspheres (HGMs) was developed in the study and its applications in buildings were extensively evaluated in China. Three types of HGMs were successfully adopted in the coating fabrications and their spectral properties were tested with the maximum albedo of 95% in the solar visible wavelength. Building energy simulation models were established based on a building prototype in typical cities located in five different thermal zones of China. The HGMs-based cool roof radiative coating with optimal albedo was integrated into the simulation model. The thermal transmission through the roof and building energy saving potential were analyzed and compared extensively with other various roof surface solar reflections and building prototypes in different climate patterns. The results showed that the optimal HGMs-based cool roof radiative coating improves the solar reflectivity by 7% and 23% in visible and near-infrared wavelength respectively when compared with traditional roof coating. For a naturally ventilated building, the HGMs-based cool roof coating is capable of achieving up to 30.9 °C cooler and a more thermally comfortable built environment than dark roof surface. For an air-conditioned building with the proposed HGMs-based cool roof coating, building cooling load savings exceed the heating energy penalties throughout the year among all five thermal zones in China, which finally induce positive net energy savings. The southern cities of Kunming and Hong Kong possess the two largest shares of energy saving rates of 8.2% and 6.3% respectively, which indicate a greater application potential of HGMs-based cool roof radiative coatings in regions with mild and hot summer & warm winter climate patterns. The new radiative coating can be integrated with building system to passively achieve energy saving and indoor thermal comfort.

**Tuesday, 20/Aug/2019 2:24pm - 2:36pm**

**Abstract ID: 348**

**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 ( $10\pm 2$  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  $1 - 3$   $\mu\text{m}$  in size were followed by the layers of fine grains of  $0.05 - 0.2$   $\mu\text{m}$  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  $500$   $\text{Sm}^{-1}$  for an interlayer with  $100$   $\mu\text{m}$  thickness and  $15$  vol.% of graphenated fibers. This value rises up to  $1000$   $\text{Sm}^{-1}$  when the fibers fraction reaches  $25$  vol.% and up to  $1700$   $\text{Sm}^{-1}$  by increasing the thickness of the layer to  $500$   $\mu\text{m}$ . 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.

Wednesday, 21/Aug/2019 1:24pm - 1:36pm

**Abstract ID: 356**

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**

**Justyna Domagała-Dubiel<sup>1</sup>, Damian Janicki<sup>2</sup>, Katarzyna Bilewska<sup>1</sup>, Wojciech Gluchowski<sup>1</sup>**

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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: 372**

**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-TiO<sub>2</sub> and Gelatin- TiO<sub>2</sub> Nanocomposites as Ethylene Scavengers for Climacteric Fruit Application**

**Jessica de Matos Fonseca<sup>1</sup>, Lenilton Santos Soares<sup>1</sup>, German Ayala Valencia<sup>1</sup>, Carlos Eduardo Maduro Campos<sup>2</sup>, Regina FPM Moreira<sup>1</sup>, Alcilene Rodrigues Monteiro Fritz<sup>1</sup>**

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Titanium dioxide (TiO<sub>2</sub>) 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, TiO<sub>2</sub> 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 TiO<sub>2</sub> [2]. This research aims to develop nanocomposite based on TiO<sub>2</sub> and hydroxypropyl methylcellulose (HPMC-TiO<sub>2</sub>) and TiO<sub>2</sub> and bovine gelatin (Gelatin-TiO<sub>2</sub>) for covering polyethylene packages used to protect fruit against injuries. It was investigated the effects of TiO<sub>2</sub> 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 TiO<sub>2</sub> nanoparticles and crystallinity, chemical composition, thermal and optical properties were changed by the incorporation of TiO<sub>2</sub> into polymer matrices. However, thickness, moisture content and hydrophilicity of HPMC and gelatin-based films did not change by the increasing of TiO<sub>2</sub> 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**

**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 concertation. 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 4:16pm - 4:28pm

**Abstract ID: 374**

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Synthesis and characterization of Composite materials

Keywords: composite, simultaneous, pollutants

### **Nanocomposite WO<sub>3</sub>-TiO<sub>2</sub> /Fly Ash With Dual Functionality In Simultaneous Removal Of Pollutants From Wastewater**

**Maria VISA**

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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 WO<sub>3</sub> and TiO<sub>2</sub> nanocrystals were obtained either by sol-gel. The TiO<sub>2</sub> and WO<sub>3</sub> 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-Cu<sup>2+</sup>. 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 (Cu<sup>2+</sup>+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, TiO<sub>2</sub> and WO<sub>3</sub> is active under VIS irradiation, proves good efficiencies in the simultaneous removal of dyes (BB, BR) and heavy metal (Cu<sup>2+</sup>). The adsorption and photocatalysis results obtained in static regime represent a starting point for continuous flow processes.

**Tuesday, 20/Aug/2019 3:36pm - 3:48pm**

**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 Magnetolectric Properties Of  $\text{BiFeO}_3\text{-CoFe}_2\text{O}_4$  Nanocomposites**

**Muneeswaran Muniyandi, Ali Akbari Fakhrabadi**

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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,  $\text{BiFeO}_3$  (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 magnetolectric 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 magnetolectric properties of BFO on addition of cobalt ferrite ( $\text{CoFe}_2\text{O}_4$ , 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 magnetolectric properties. Nanocomposites consisting of BFO and CFO, with composition range of  $(1-x) \text{BiFeO}_3\text{-}x\text{CoFe}_2\text{O}_4$ , where  $x = 0.10, 0.20, 0.30$  and  $0.40$  have been prepared by the hydrothermal method. Structural, magnetic, vibrational and magnetolectric properties of the prepared nanocomposites have been studied in detail to understand the role of CFO in modifying magnetolectric properties of BFO. To explore the coupling between the magnetic and ferroelectric properties at room temperature for multi ferroic  $(1-x) \text{BiFeO}_3\text{-}x\text{CoFe}_2\text{O}_4$ , ( $x=0.10, 0.20, 0.30$  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.

**References**

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**Abstract ID: 446**

**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.

**Abstract ID: 463**

**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 1:12pm - 1:24pm

**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**

**Stephen Agwuncha<sup>1</sup>, Shesan Owonubi<sup>2</sup>, Neerish Revaprasadu<sup>2</sup>**

<sup>1</sup>Ibrahim Badamasi Babangida University, Lapai, Nigeria, Nigeria; <sup>2</sup>Department of Chemistry, University of Zululand, Kwadlangezwa, Kwazulu Natal, RSA; [agwunchas@ibbu.edu.ng](mailto:agwunchas@ibbu.edu.ng)

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 NaClO<sub>2</sub>, as bleaching agent, further removed the hemicelluloses remaining in the samples as observed in the TGA. 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 liquor 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.

**Tuesday, 20/Aug/2019 3:12pm - 3:24pm**

**Abstract ID: 479**

**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**

**Jacek Wladyslaw Kaczmar, Krzysztof Naplocha, Anna Dmitruk, Jakub Grzeda**

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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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Tuesday, 20/Aug/2019 2:48pm - 3:00pm

**Abstract ID: 487**

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/Fe<sub>3</sub>O<sub>4</sub>@C, Via In Situ Carbonization of Fe<sub>3</sub>O<sub>4</sub>-Lignin Framework**

**Chenglong Yuan<sup>1</sup>, Zhichao Lou<sup>1,2</sup>, Yao Zhang<sup>1</sup>, Weikai Wang<sup>1</sup>, Lintian Yang<sup>1</sup>, Yanjun Li<sup>1</sup>**

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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/Fe<sub>3</sub>O<sub>4</sub>/Fe composites (GFF) by carbonizing Fe<sub>3</sub>O<sub>4</sub>-lignin frameworks which were prepared through a two-step carbodiimide coupling protocol. The in-depth investigation confirmed the composites were Fe/Fe<sub>3</sub>O<sub>4</sub> 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/Fe<sub>3</sub>O<sub>4</sub> 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/Fe<sub>3</sub>O<sub>4</sub> 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.

Wednesday, 21/Aug/2019 6:04pm - 6:16pm

**Abstract ID: 508**

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

**Michael Shtein, Roey Nadiv, Matat Buzaglo, Oren Regev**

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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**

**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**

**Matan Birenboim**

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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.

Wednesday, 21/Aug/2019 1:48pm - 2:00pm

**Abstract ID: 512**

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**

**Shanyu Meng, Arianna Partow, zhaohui Tong**

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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 <sup>13</sup>C-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: 514**

**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**

**Junhyung Kim<sup>1,2</sup>, Yujin Hwang<sup>1,2</sup>, Sunho Jeong<sup>1</sup>, Su Yeon Lee<sup>1</sup>, Youngmin Choi<sup>1,2</sup>, Sungmook Jung<sup>1</sup>**

<sup>1</sup>Korea Research Institute of Chemical Technology; <sup>2</sup>Department of Chemical Convergence Materials, Korea University of Science and Technology; [mooktank@kriict.re.kr](mailto:mooktank@kriict.re.kr)

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.<sup>1,2</sup> 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<sup>-1</sup>), Young's modulus (16–535 kPa), and stretchability (430–1340%) while durability was maintained (stable upto 10,000 stretching cycles at 100% strain).<sup>2</sup> 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: 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<sup>1,2</sup>, Guicai Qi<sup>1,2,3</sup>, Yuan Zhou<sup>1,2</sup>, Yue Shen<sup>1,2</sup>, Yanxia Sun<sup>1,2</sup>, Shengde Dong<sup>1,2,3</sup>, Xiang Li<sup>1,2</sup>**

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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  $\text{Mn}_2\text{O}_3$  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.

Wednesday, 21/Aug/2019 4:28pm - 4:40pm

**Abstract ID: 530**

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

*Topics:* Synthesis and characterization of Composite materials

*Keywords:* MOFs (metal-organic framework); self-assembly; MoS<sub>2</sub>; composites; CO<sub>2</sub> adsorption

### Self-assembly Composites of HKUST-1 MOFs with MoS<sub>2</sub> for CO<sub>2</sub> adsorption

**Xueliang Mu, Shuai Liu, Yipei Chen, Tao Wu**

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Novel ordered composites comprised of micropores and mesopores were synthesized by assembling HKUST-1 on MoS<sub>2</sub> nanosheet. The MoS<sub>2</sub>/HKUST-1 was characterized using a combination of XRD, TEM, SEM, TPD, BET, CO<sub>2</sub> adsorption test, respectively. In this study, the amount of MoS<sub>2</sub> cores was demonstrated to influence the adsorption performance. The results suggest that the co-existence of MoS<sub>2</sub> could promote the formation of minimized-scale HKUST-1, and the addition of MoS<sub>2</sub> does not affect HKUST-1 structure. Furthermore, the micropore/mesopore volume ratio can be controlled by varying the amount of MoS<sub>2</sub> used. The CO<sub>2</sub> adsorption capacities were examined by CO<sub>2</sub> adsorption isotherm at 25°C. The CO<sub>2</sub> adsorption capacity of modified HKUST-1 reaches 21.21 wt%. All the original/modified HKUST-1 remain high CO<sub>2</sub> uptake in 10 times of adsorption/desorption cycles.

Wednesday, 21/Aug/2019 2:12pm - 2:24pm

**Abstract ID: 539**

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**

**Nikolai Stoyanov Boshkov<sup>1</sup>, Neli Dimitrova Boshkova<sup>1</sup>, Kamelia Pavlova Kamburova<sup>1</sup>, Nadezhda Vladimirova Tabakova<sup>2</sup>, Tsetska Borisova Radeva<sup>1</sup>**

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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 2:48pm - 3:00pm

**Abstract ID: 542**

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**

**Xiaojing Liu, Yangcheng Lu**

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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 Fe<sub>3</sub>O<sub>4</sub>, 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 Fe<sub>3</sub>O<sub>4</sub> 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.

Wednesday, 21/Aug/2019 3:12pm - 3:24pm

**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**

**Roberta Sburlati, Roberto Cianci**

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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: 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**

Qinghai Institute of Salt Lakes, Chinese Academy of Sciences, Xining, China; [lixiang@isl.ac.cn](mailto:lixiang@isl.ac.cn)

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.

**Tuesday, 20/Aug/2019 4:00pm - 4:12pm**

**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**

**Xu Wu, Yichun Zhang**

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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.<sup>1-3</sup> 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: 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**

**Taehee Kim, Miri Kim, Wonjoo Lee, Choong-Sun Lim, Bongkuk Seo**

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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.

Wednesday, 21/Aug/2019 2:12pm - 2:24pm

**Abstract ID: 565**

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**

**Thollwana Makhetha, Richard Motlhaletsi Moutloali**

University of Johannesburg, South Africa; [rmoutloali@uj.ac.za](mailto:rmoutloali@uj.ac.za)

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 m<sup>2</sup> g<sup>-1</sup> with a pore volume of 0.0069 m<sup>3</sup> g<sup>-1</sup> 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<sup>-1</sup> 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.

Wednesday, 21/Aug/2019 1:36pm - 1:48pm

**Abstract ID: 569**

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**

**Mei Chee Tan<sup>1</sup>, Xinyu Zhao<sup>1</sup>, Yang Sun<sup>2</sup>, George Chen<sup>1</sup>, Chaobin He<sup>2,3</sup>, Dawn Tan<sup>1</sup>**

<sup>1</sup>Singapore University of Technology and Design, Singapore; <sup>2</sup>National University of Singapore, Singapore; <sup>3</sup>Institute of Materials Research and Engineering, Agency for Science, Technology and Research (A\*STAR); [meichee.tan@sutd.edu.sg](mailto:meichee.tan@sutd.edu.sg)

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 NaYF<sub>4</sub> 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-SiO<sub>2</sub> 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  $\sim 0.58$  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.

Wednesday, 21/Aug/2019 4:04pm - 4:16pm

**Abstract ID: 587**

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.

Wednesday, 21/Aug/2019 5:52pm - 6:04pm

**Abstract ID: 605**

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 Smearred Peristaltic Fluid Pumps**

**Eduard Rohan, Vladimír Lukeš, Jan Heczko**

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Fluid transport in porous materials can be assisted by the fluid-structure interactions due 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, 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 smearred 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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**Tuesday, 20/Aug/2019 1:12pm - 1:24pm**

**Abstract ID: 617**

**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**

**Wusheng Fan<sup>1,2</sup>, Ni Feng<sup>1</sup>, Guangming Chen<sup>2</sup>, Lirong Liang<sup>1</sup>, Cun-Yue Guo<sup>1</sup>**

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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.<sup>1–5</sup> Therefore, we prepared three types of flexible single-walled carbon nanotube (SWCNT)-based TE composites (polypyrrole/SWCNT (PPy/SWCNT) nanocomposites,<sup>1,2</sup> copper-phenylacetylide/SWCNT (PhC2Cu/SWCNT) nanocomposites,<sup>3</sup> and poly(3,4-ethylenedioxythiophene)/SWCNT (PEDOT/SWCNT) nanocomposites<sup>5</sup>) 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.

Wednesday, 21/Aug/2019 2:24pm - 2:36pm

**Abstract ID: 630**

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**

**Zhichuan Tang<sup>1</sup>, Zhengsong Qiu<sup>1</sup>, Hanyi Zhong<sup>1</sup>, Baoyu Guo<sup>2</sup>, Xudong Wang<sup>2</sup>, Yujie Kang<sup>1</sup>**

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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: 632**

**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**

**Natalia Stachowiak, Justyna Kozłowska, Halina Kaczmarek**

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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.

Wednesday, 21/Aug/2019 3:24pm - 3:36pm

**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**

**Harmaen Ahmad Saffian<sup>1</sup>, Mohd Aizam Talib<sup>2</sup>, Ainun Zuriyati Mohamad Asa'ari<sup>1</sup>, Paridah Md Tahir<sup>1</sup>, Seng Hua Lee<sup>1</sup>**

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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: 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**

**Anjali Panwar<sup>1</sup>, Vikas Malik<sup>2</sup>, Neeleshwar Sonnathi<sup>1</sup>, Anjana Bagga<sup>1</sup>**

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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 1:24pm - 1:36pm

**Abstract ID: 675**

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

**Tuesday, 20/Aug/2019 1:00pm - 1:12pm**

**Abstract ID: 693**

**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**

**Paula Ferreira**

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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-Fe<sub>3</sub>-xO<sub>4</sub>) filler in different percentages. The filler is prepared by one-pot synthesis, ensuring good dispersibility of the Fe<sub>3</sub>-xO<sub>4</sub> 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-Fe<sub>3</sub>-xO<sub>4</sub> film. Furthermore, the composites are cytocompatibles with HaCat cell lines.

Wednesday, 21/Aug/2019 2:24pm - 2:36pm

**Abstract ID: 706**

Symposium 2: Functional Composite Materials (FCM)

Plenary

*Topics:* Composite structural materials

*Keywords:* Ti/Al<sub>2</sub>O<sub>3</sub> composites; sintering aid; mechanical properties

**Fabrication And Mechanical Properties Of Ti/Al<sub>2</sub>O<sub>3</sub> Composites With CeO<sub>2</sub>, Y<sub>2</sub>O<sub>3</sub>,  
And ZrO<sub>2</sub> Doped**

**Guopu Shi, Liu Zhang, Zhi Wang, Qinggang Li, Junyan Wu**

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Ti/Al<sub>2</sub>O<sub>3</sub> composites doped with CeO<sub>2</sub>, Y<sub>2</sub>O<sub>3</sub>, and ZrO<sub>2</sub> 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/Al<sub>2</sub>O<sub>3</sub>-CeO<sub>2</sub> composites have been demonstrated being endowed the best mechanical properties with the porosity of 19.33%, bending strength of  $178.26 \pm 2.14$  MPa, and fracture toughness of  $2.53 \pm 0.11$  MPa·m<sup>1/2</sup>, respectively, which was attributed to the contribution of tough phase CeAlO<sub>3</sub>. Fracture toughness and bending strength have both increased upon 20% than these of Ti/Al<sub>2</sub>O<sub>3</sub> composites. Meanwhile, the toughening mechanism has been studied via analyzing the microstructure and phase component.

Wednesday, 21/Aug/2019 1:36pm - 1:48pm

**Abstract ID: 710**

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, and sintering parameters, to identify the best suitable combinations to fabricate various porous structures. The fabricated workpieces are then observed by SEM to understand the binding of the fused particles; the density, surface roughness, and shrinkage rate were calculated.

Tuesday, 20/Aug/2019 3:00pm - 3:12pm

**Abstract ID: 756**

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

**Neeleshwar Sonnathi<sup>1</sup>, Bayikadi Khasimsaheb<sup>1</sup>, Sivaiah Bathula<sup>2</sup>, Yang-Yuan Chen<sup>3</sup>, Sriparna Bhattacharya<sup>4</sup>, Apparao M. Rao<sup>4</sup>**

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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)<sub>0.89</sub>(AgSbTe<sub>2</sub>)<sub>0.1</sub>(SnSe)<sub>0.01</sub> 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.

Wednesday, 21/Aug/2019 1:12pm - 1:24pm

**Abstract ID: 757**

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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Tuesday, 20/Aug/2019 1:36pm - 1:48pm

**Abstract ID: 761**

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

**Fabrizio Giovanni Ezio Verga<sup>1</sup>, Alexandre Staub<sup>1</sup>, Manfred Schmid<sup>1</sup>, Konrad Wegener<sup>2</sup>**

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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 ( $\lambda$ ) of 1.064  $\mu\text{m}$  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  $\mu\text{m}$ ). 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: 768**

**Symposium 2: Functional Composite Materials (FCM)**

**Poster Presentation**

*Topics:* Nanocomposites

*Keywords:* N-ZnONCBs Catalyst, Hydrothermal Method, Photodegradation, Methylene blue, 2, 4-DCP, UV light and Visible light irradiation

### **Efficient Photocatalytic Degradation of Methylene Blue and 2,4-DCP under UV and Visible light**

**Eswaran Prabakaran, Kriveshini Pillay**

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In this study, the synthesis of nitrogen-doped zinc oxide nanoparticles with a cabbage like morphology (N-ZnONCBs) by a hydrothermal method using zinc acetate dihydrate as a precursor and hydrazine monohydrate as a nitrogen source is reported. N-ZnONCBs was characterized using UV-visible Spectroscopy (UV-Vis), Fluorescence Spectroscopy, Fourier Transmittance Infrared Spectroscopy (FTIR), X-ray diffraction (XRD), Raman Spectroscopy, Thermogravimetric Analysis (TGA), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Electron Dispersive Spectroscopy (EDS) and EDX elemental mapping. N-ZnONCBs were tested for their photocatalytic capabilities in the degradation of methylene blue (MB) under UV-light and visible light irradiation. The N-ZnONCBs catalyst demonstrated improved photodegradation efficiency (98.6 % and 96.2 %) and kinetic degradation rates of MB ( $k = -0.0579 \text{ min}^{-1}$  and  $k = -0.0585 \text{ min}^{-1}$ ) under UV light and visible light irradiation. The photocatalytic degradation intermediate products were obtained by Liquid chromatography mass spectra (LC-MS) and also complete mineralization was determined by using Total Organic Carbon (TOC) studies. This photocatalyst was also tested with 2,4-Dichlorophenol (2,4-DCP) under visible light irradiation at different time intervals. Fluorescence and quenching studies were performed for the binding interaction between N-ZnONCBs catalyst and MB dye. The N-ZnONCBs catalyst was also tested for its photostability and reusability with a percentage degradation rate of MB (93.2 %) after 4 cycle experiments. These results have clearly demonstrated that N-ZnONCBs catalyst can be applied for the photocatalytic degradation of MB from wastewater samples.

Wednesday, 21/Aug/2019 3:12pm - 3:24pm

**Abstract ID: 779**

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: MoS<sub>2</sub>/Ag, MoS<sub>2</sub>/ZnO, Nanocomposites, Photocatalysis

### MoS<sub>2</sub> Based Nanocomposites for Photocatalytic Degradation of Industrial Dyes

**Akshay Kumar, Unni Krishnan, Manjot Kaur**

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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 (MoS<sub>2</sub>) possess unique properties such as direct band gap and sandwich molecular layered structure which makes it suitable as photocatalyst. However, MoS<sub>2</sub> 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, MoS<sub>2</sub> based nanocomposites (MoS<sub>2</sub>/ZnO and MoS<sub>2</sub>/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. MoS<sub>2</sub>/Ag (30%) photocatalyst with 1g/L concentration results in ~78% degradation whereas MoS<sub>2</sub>/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 MoS<sub>2</sub> based nanocomposites a favorable photocatalyst for degradation of industrial pollutants.

**Tuesday, 20/Aug/2019 1:48pm - 2:00pm**

**Abstract ID: 787**

**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**

**Zhihe Jin**

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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.

Wednesday, 21/Aug/2019 2:36pm - 2:48pm

**Abstract ID: 795**

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

**Xiao-Zhang Zhang**

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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 Kirchoff'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: 808**

**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**

**Sheng Yih Luo, Yu Hsiang Chung, Cheng Ru Wu**

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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.

Tuesday, 20/Aug/2019 2:12pm - 2:24pm

**Abstract ID: 819**

Symposium 2: Functional Composite Materials (FCM)

Oral Presentation

Topics: Nanocomposites

Keywords: Carbon nanotube yarn, stretching, twisting, tetrabromoaurate (KAuBr<sub>4</sub>)

### Highly Conductive Carbon Nanotube Yarns with Improved Strength

**Igor Maria De Rosa, Wenbo Xin, Larry Carlson**

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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 tetrabromoaurate (KAuBr<sub>4</sub>). 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 1.0x10<sup>5</sup>±0. 2x10<sup>4</sup> S/m (pristine) to 1.2±0.1 GPa, 49.3±5.2 GPa, and 1.8x10<sup>6</sup>±7x10<sup>4</sup> 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].

Wednesday, 21/Aug/2019 3:40pm - 3:52pm

**Abstract ID: 836**

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**

**Yu Hou<sup>1</sup>, Jimei Qi<sup>1</sup>, Jiwei Hu<sup>1</sup>, Fei Huang<sup>2</sup>, Wenqian Ruan<sup>1</sup>, Yiqiu Xiang<sup>1</sup>, Xionghui Wei<sup>3</sup>**

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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, N<sub>2</sub>-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 m<sup>2</sup>/g, a single point adsorption total pore volume of 0.4783 cm<sup>3</sup>/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 R<sup>2</sup> 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 (R<sup>2</sup> 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<sup>-1</sup> and 0.0322 kJ mol<sup>-1</sup> K<sup>-1</sup>, 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: 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**

**Shuyu Ni, Yan Jiang, Jialei Yuan, Xumin Gao, Zheng Shi, yongjin wang**

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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- $\mu\text{m}$ -wide and 155- $\mu\text{m}$ -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  $\lambda$  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].

Wednesday, 21/Aug/2019 3:00pm - 3:12pm

**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: 886**

**Symposium 2: Functional Composite Materials (FCM)**

**Poster Presentation**

*Topics:* Applications of Composites

*Keywords:* Composite nanofibers; Chitosan; Electrospinning; Efficient Adsorption; Pb(II) and Cd(II) ions.

### **Electrospun Composite Nanofiber Membranes of Poly(Vinyl Alcohol)/Chitosan For Selective Lead(II) And Cadmium(II) Ions Removal From Wastewater**

**sahar saad shar, Mohammad Rezaul Karim**

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The poly(vinyl alcohol)/chitosan (PVA/Chi) nanofibers membranes were fabricated by using an electro-spun technique for selective and high adsorption of lead (Pb(II)) and cadmium (Cd(II)) ions based on the solution acidity. The adsorption were depends on many factors such as initial metal ions concentration, interaction time, adsorbent dosage, solution pH of both ions Pb(II) and Cd(II). The adsorption data were also clarified that the PVA/Chi NFs membranes were exhibited high kinetic performances towards the both toxic ions at the optimum conditions. The adsorption data were manipulated using different kinetics models, and it was confirmed that only pseudo-second-order model obeyed the adsorption kinetics for Pb(II) and Cd(II) ions. Similarly, the equilibrium data were well fitted with the Langmuir adsorption isotherms model, and the maximum adsorption capacity was 266.12 and 148.79 mg/g for Pb(II) and Cd(II) ions, respectively. the data were confirming the high selectivity to Pb(II) and Cd(II) ions at the optimum condition and the nanofibers membrane proved as efficient methods for removal of the selected toxic ions from waste samples. Thus, the PVA/Chi NFs are promising materials for Pb(II) and Cd(II) ions from wastewaters with high efficiency.

**Tuesday, 20/Aug/2019 10:50am - 11:20am**

**Abstract ID: 894**

**Symposium 2: Functional Composite Materials (FCM)**

**Keynote**

*Topics:* Polymeric composites

*Keywords:* conducting polymer, polyaniline, nanofibers, membrane, antifouling

### **Conjugated Nanostructured Polyaniline for Emergent Membrane Technologies**

**Richard B. Kaner**

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Polyaniline, in the family of conjugated polymers, has emerged as an ideal functional material for numerous applications. Its ease of synthesis and processability will spur even more technological advances in the field. In particular, polyaniline in its nanostructured form as nanofibers can be produced through template-free and readily scalable methods using interfacial polymerization or rapidly mixing aniline, oxidant and acid.[1-3] We have found that the formation of nanofibers requires suppression of secondary growth and the facilitation of heterogeneous nucleation.[4] Polyaniline nanofibers can be used as chemiresistors, mechanical actuators (artificial muscles), catalysts and volatile memory devices.[1,5-7] Recently, polyaniline has drawn our attention with its superior performance for membrane filtration technologies due to its hydrophilic nature.[8] Incorporation of functionalized polyaniline nanofibers into ultrafiltration membranes can lead to low fouling and chlorine tolerant properties[9,10] This has been further demonstrated by blending carbon nanotubes or sulfonated self-doped polyaniline into polysulfone to significantly improve hydrophilicity of the ultrafiltration membranes, further enhancing fouling resistance. Another way of tuning flux and selectivity of the membrane is by adding carbon nanotubes and applying flash welding which takes advantage of polyaniline nanofibers' high photothermal conversion efficiency.[11,12]

# **SYMPOSIUM 3: Functional Catalysis (FC)**

Wednesday, 21/Aug/2019 6:52pm - 7:04pm

**Abstract ID: 154**

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**

**Sungjin Park**

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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.

Wednesday, 21/Aug/2019 6:16pm - 6:28pm

**Abstract ID: 163**

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@TiO<sub>2</sub> 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@TiO<sub>2</sub> core-shell nanoparticles (NPs). Stable to oxidation Ti@TiO<sub>2</sub> 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@TiO<sub>2</sub> 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@TiO<sub>2</sub> 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@TiO<sub>2</sub> NPs exhibit much higher photocatalytic activity in H<sub>2</sub> production from aqueous solutions of glycerol (40 % vol.) under vis/NIR light compared to pristine anatase TiO<sub>2</sub> or air-passivated Ti NPs. In addition, Ti@TiO<sub>2</sub> NPs show strong photothermal effect providing the most efficient H<sub>2</sub> production under the joint effect of light and heat. The apparent activation energy  $E_a = 27$  kJ·mol<sup>-1</sup> assumes that the thermal effect of H<sub>2</sub> 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 TiO<sub>2</sub> shell via charge separation and multiple charge-transfer steps. The photoluminescence of TiO<sub>2</sub> originated from electron-hole recombination is completely quenched in the case of Ti@TiO<sub>2</sub> NPs indicating effective charge separation. In principal, Ti@TiO<sub>2</sub> photocatalyst has the same potential areas of applications as TiO<sub>2</sub>/Pt photocatalyst.

Wednesday, 21/Aug/2019 6:28pm - 6:40pm

**Abstract ID: 206**

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**

**Ha-Young Lee<sup>1</sup>, Chunfei Zhang<sup>1,2</sup>, Cheol-hwan Shin<sup>1</sup>, Jong-Sung Yu<sup>1</sup>**

<sup>1</sup>Daegu Gyeongbuk Institute of Science and Technology (DGIST), Korea, Republic of (South Korea); <sup>2</sup>Faculty of Maritime and Transportation, Ningbo University, Ningbo 315832, China; [jsyu@dgist.ac.kr](mailto:jsyu@dgist.ac.kr)

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 Au<sup>3+</sup>, Pt<sup>4+</sup>, Ag<sup>+</sup>, and Cu<sup>2+</sup> (M<sup>x+</sup>) to MNPs on the graphene to form G/MNP composites.<sup>1</sup> 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)<sub>2</sub> nanosheets is also elucidated. Ni(OH)<sub>2</sub>-wrapped Ag hybrid developed on the GNF (Ag@Ni(OH)<sub>2</sub>-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.

Wednesday, 21/Aug/2019 5:28pm - 5:40pm

**Abstract ID: 236**

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 CO<sub>2</sub> 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 CO<sub>2</sub> 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 CO<sub>2</sub> 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 CO<sub>2</sub> reduction under solar light and the 3D core-shell electrocatalysts significantly advance the study for large-scale practical water electrolysis.

Wednesday, 21/Aug/2019 4:04pm - 4:16pm

**Abstract ID: 259**

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**

**Ying Zhu**

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The electrocatalytic conversion of renewable resources, such as electrical energy, CO<sub>2</sub> 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 CO<sub>2</sub> 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 CO<sub>2</sub> to ethanol, overcoming the usual limitation of low faradaic efficiencies and selectivity for C<sub>2</sub> products. The hydrophobic exfoliated MoS<sub>2</sub> (H-E-MoS<sub>2</sub>) nanosheets are fabricated from bulk MoS<sub>2</sub> by a cost-effective ball-milling method, followed by decoration with fluorosilane. H-E-MoS<sub>2</sub> as cost-effective electrocatalyst is capable to directly reduce CO<sub>2</sub> and H<sub>2</sub>O to tunable syngas production with a wide range of CO/H<sub>2</sub> ratio from 1:2 to 4:1.

Wednesday, 21/Aug/2019 6:04pm - 6:16pm

**Abstract ID: 328**

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalysis for pollution control

Keywords: Photocatalysis, Vanadium pentoxide, Wastewater decolourization

### **Hemin (Fe<sup>+3</sup>-Porphyrin) Anchored V<sub>2</sub>O<sub>5</sub> Nanowires for Solar Light Based Photocatalytic Decolourization of MB Dye and Industrial Wastewater**

**Pankaj Singh Chauhan, Shantanu Bhattacharya**

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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 (V<sub>2</sub>O<sub>5</sub>) 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<sup>-</sup>) at the valence band of V<sub>2</sub>O<sub>5</sub> gets excited and jump to the conduction band and leave holes (h<sup>+</sup>) behind at the valence band. These electrons and holes react with water molecules and form hydroxyl radical (OH•), which is a highly reactive oxidizing agent and degrades complex dye molecules. Although, V<sub>2</sub>O<sub>5</sub> 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 V<sub>2</sub>O<sub>5</sub> nanostructures. Hemin (Fe<sup>+3</sup>-porphyrin) is an iron containing compound which shows excellent solar light trapping property. Hemin, anchored with V<sub>2</sub>O<sub>5</sub> serves dual function by providing a conducting path for electrons present at the conduction band of V<sub>2</sub>O<sub>5</sub> 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 V<sub>2</sub>O<sub>5</sub> nanowires (H-V<sub>2</sub>O<sub>5</sub>) 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-V<sub>2</sub>O<sub>5</sub> in comparison with pure V<sub>2</sub>O<sub>5</sub> for MB dye. H-V<sub>2</sub>O<sub>5</sub> 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 V<sub>2</sub>O<sub>5</sub> 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-V<sub>2</sub>O<sub>5</sub> as an efficient photo-catalyst for MB and wastewater dye decolourization utilizing the solar light as a source of energy.

Thursday, 22/Aug/2019 1:30pm - 1:42pm

**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**

**Kyriakos Stylianou**

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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,  $\text{NH}_3\text{BH}_3$ ). SION-X is the synthetic form of a mineral and, following in situ reduction, catalyzes the release of almost all 3 equivalents of hydrogen ( $\text{H}_2$ ) 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  $\text{H}_2$  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.

Wednesday, 21/Aug/2019 4:16pm - 4:28pm

**Abstract ID: 355**

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

**Elisabete Alegria<sup>1,2</sup>, Ana Ribeiro<sup>2</sup>, Maximilian Kopylovich<sup>2</sup>, Armando Pombeiro<sup>2</sup>**

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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.

Wednesday, 21/Aug/2019 4:40pm - 4:52pm

**Abstract ID: 365**

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Photocatalysis

Keywords: Photocatalysis, CO<sub>2</sub> reduction, DFT simulations

### Silicon Nanoparticles-based Photocatalysts for Efficient CO<sub>2</sub> Reduction

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Solar-driven hydrogenation of CO<sub>2</sub> 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 CO<sub>2</sub> 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 mechanism<sup>1</sup>. Next, we will discuss enhancing this catalyst activity by supporting this silicon photonic crystal by ruthenium, which results into CO<sub>2</sub> reduction rates as large as  $2.8 \text{ mmol h}^{-1} \text{g}^{-1}$  at ambient temperature; and the corresponding atomistic mechanism underpinning this reaction<sup>2</sup>. The results from the DFT simulations indicate that charged Ru surfaces can destabilize adsorbed CO<sub>2</sub> molecules and adsorb and dissociate H<sub>2</sub> such that it can readily react with CO<sub>2</sub>, 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.

**Abstract ID: 397**

**Symposium 3: Functional Catalysis (FC)**

**Poster Presentation**

*Topics:* Nano and Environmental catalysis

*Keywords:* Nanoporous MOF materials, Organic linkers, Lewis basic nitrogen sites, CO<sub>2</sub> Capture, Catalysis

## **Nanoporous Metal Organic Frameworks for CO<sub>2</sub> capture and Heterogeneous Catalysis**

**Thirunarayanan Ayyavu, Monica Soler, Francisco Gracia**

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Nanoporous Metal Organic Frameworks for CO<sub>2</sub> 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,<sup>1,2</sup> 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.<sup>3,4</sup> Rational design of basic active centers allows one to substantially improve the catalytic performance,<sup>5</sup> in particular, to enhance the activity and selectivity along with CO<sub>2</sub> 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 CO<sub>2</sub> 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 benzothiazole<sup>5</sup> derivatives. The MOFs are thoroughly characterized by using a variety of techniques such as (XRD), (FT-IR), (AAS),(TGA), (SEM), (TEM) and N<sub>2</sub>-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 in to 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, CO<sub>2</sub> Capture, Catalysis.

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Wednesday, 21/Aug/2019 7:04pm - 7:16pm

**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  $\text{Cu}^{2+}$  was synthesized. The  $\text{Cu}^{2+}$ -chelated MGO (MGO- $\text{Cu}^{2+}$ ) 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- $\text{Cu}^{2+}$  was 114%. The catalytic properties of MGO- $\text{Cu}$ -CotA laccase were significantly improved in comparison with those of free laccase. MGO- $\text{Cu}$ -CotA laccase showed efficient decolorization rate for Congo red reached 100% after 5 h reaction at 60 °C and pH 8. MGO- $\text{Cu}$ -CotA laccase retained 89.4 % of its initial activity after 10 consecutive cycles. These MGO- $\text{Cu}^{2+}$  supports provide great potential for large-scale laccase immobilization in practice. [4]

**Wednesday, 21/Aug/2019 6:40pm - 6:52pm**

**Abstract ID: 462**

**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-C<sub>3</sub>N<sub>4</sub> prepared at 510 °C nor in g-C<sub>3</sub>N<sub>4</sub> 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.

Wednesday, 21/Aug/2019 7:16pm - 7:28pm

**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**

**Tiexin Zhang, Chunying Duan**

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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 CF<sub>3</sub> 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.

Wednesday, 21/Aug/2019 5:40pm - 5:52pm

**Abstract ID: 531**

Symposium 3: Functional Catalysis (FC)

Oral Presentation

Topics: Catalysis for pollution control

Keywords: g-C<sub>3</sub>N<sub>4</sub>; mercury removal; single-atom catalyst; Mn

**Carbon nitride-support Single Mn atom as catalyst for Mercury removal in flue gas by first-principles calculations**

**Shuai Liu, Xueliang Mu, Jiahui Yu, Gang Yang, Xiang Luo, Haitao Zhao, Mengxia Xu, Tao Wu**

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Elemental mercury(Hg<sup>0</sup>) 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-C<sub>3</sub>N<sub>4</sub>-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-C<sub>3</sub>N<sub>4</sub> 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 Hg<sup>2+</sup> under O<sub>2</sub> takes place through the E-R mechanism, where O<sub>2</sub> competes for Mn site with Hg<sup>0</sup> and breaks down easily with the existence of mercury, later connecting the gas phase or a weakly adsorbed Hg<sup>0</sup>. This study offers a promising guide of single-atom catalysts to significantly improve the efficiency of the control of mercury pollution with g-C<sub>3</sub>N<sub>4</sub>-based support effects.

Wednesday, 21/Aug/2019 5:52pm - 6:04pm

**Abstract ID: 550**

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**

**Jian-Wen Shi, Dandan Ma, Yajun Zou**

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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-C<sub>3</sub>N<sub>4</sub>/C-TiO<sub>2</sub> hollow structures, In<sub>2</sub>S<sub>3</sub>/CdIn<sub>2</sub>S<sub>4</sub>/In<sub>2</sub>O<sub>3</sub>, 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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Wednesday, 21/Aug/2019 5:04pm - 5:16pm

**Abstract ID: 594**

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**

**Balasubramanian Sengottuvelan, Abiraman Tamilselvan, Rajavelu Kannan, Rajakumar Perumal**

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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

Wednesday, 21/Aug/2019 5:16pm - 5:28pm

**Abstract ID: 604**

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-NH<sub>2</sub> under Visible Light Irradiation**

**Stavroula Alina Kampouri, Kyriakos C. Stylianou**

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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-NH<sub>2</sub> is first systematically studied. All co-catalyst/MIL-125-NH<sub>2</sub> photocatalytic systems are found to be highly stable after photocatalysis, with the NiO/MIL-125-NH<sub>2</sub> and Ni<sub>2</sub>P/MIL-125-NH<sub>2</sub> systems exhibiting high hydrogen (H<sub>2</sub>) evolution rates of 1084 and 1230  $\mu\text{mol h}^{-1} \text{g}^{-1}$ , respectively. Second, how different electron donors affect the stability and H<sub>2</sub> generation rate of the best Ni<sub>2</sub>P/MIL-125-NH<sub>2</sub> 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 H<sub>2</sub> 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 H<sub>2</sub> 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 H<sub>2</sub> is produced, captured and further utilized.

Wednesday, 21/Aug/2019 4:28pm - 4:40pm

**Abstract ID: 651**

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**

**Mohamed-Nawfal Ghazzal, Cong Wang, Hynd Remita, Christophe Colbeau-Justin**

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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, TiO<sub>2</sub> 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: 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  $\text{TiO}_2$  using hybrid functional and DFT+U methods**

**Jeffrey Roshan De Lile<sup>1</sup>, Young-A Son<sup>2</sup>, Seung Geol Lee<sup>1</sup>**

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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**

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**Abstract ID: 701**

**Symposium 3: Functional Catalysis (FC)**

**Poster Presentation**

*Topics:* Catalysis for Chemical Synthesis

*Keywords:* Metallo porphyrin, TiO<sub>2</sub>, Rhodamine, Visible light, Photocatalysis, Photodegradation

**Study on Visible Light Photo-Sensitized Metallo-Porphyrin/TiO<sub>2</sub> and its Photocatalytic Activities**

**Gisu Heo<sup>1</sup>, Ramalingam Manivannan<sup>1</sup>, Hyorim Kim<sup>1</sup>, Ji Won Ryu<sup>1</sup>, Seung Geol Lee<sup>2</sup>,  
Young-A Son<sup>1</sup>**

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Organic dye degrading property in Poly Ethylene Terephthalate polymer through photo catalytic effect by metallo porphyrin and TiO<sub>2</sub> has been studied in details. The surface has been modified by step wise deposition of anatase TiO<sub>2</sub> 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 TiO<sub>2</sub> 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.

Wednesday, 21/Aug/2019 4:52pm - 5:04pm

**Abstract ID: 717**

Symposium 3: Functional Catalysis (FC)

Oral Presentation

*Topics:* Catalysis for pollution control

*Keywords:* Visible light photocatalysis, Carbon quantum dots (CDs), Ti<sup>3+</sup> and nitrogen co-doped TiO<sub>2</sub>, CDs-N-TiO<sub>2-x</sub>, photoreduction of Cr(VI)

**Facial Fabrication Of Carbon Quantum Dots (Cds)-Modified N-TiO<sub>2-x</sub>  
Nanocomposite For The Efficient Photoreduction Of Cr(VI) Under Visible Light**

**Lu Xu, Xue Bai, Pengkang Jin**

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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<sub>2-x</sub> nanocomposite was successfully fabricated by decorating the carbon quantum dots (CDs) on the nitrogen (N) and Ti<sup>3+</sup> co-doped TiO<sub>2</sub> nanoparticles using a facile hydrothermal-calcination method. The crystal structure, morphology, optical property, and chemical composition of the CDs-N-TiO<sub>2-x</sub> nanocomposite were investigated via several characterizations. Owing to the synergy between the modification of CDs and co-doping of N and Ti<sup>3+</sup>, the as-prepared CDs-N-TiO<sub>2-x</sub> nanocomposite exhibited enhanced visible light absorption and more efficient charge separation compared with its counterparts, such as the pristine TiO<sub>2</sub>, N-doped TiO<sub>2</sub> (N-TiO<sub>2</sub>), N and Ti<sup>3+</sup> codoped TiO<sub>2</sub> (N-TiO<sub>2-x</sub>), and carbon quantum dots-TiO<sub>2</sub> (CDs-TiO<sub>2</sub>), etc. As a result, the CDs-N-TiO<sub>2-x</sub> 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<sub>2-x</sub> nanocomposite. The mechanism of the enhanced photoreduction of Cr(VI) by the CDs-N-TiO<sub>2-x</sub> nanocomposite was discussed based on all the characterization and experimental results. Moreover, the developed CDs-N-TiO<sub>2-x</sub> 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<sub>2-x</sub> for the treatment of Cr(VI)-containing wastewater.

**Abstract ID: 764**

**Symposium 3: Functional Catalysis (FC)**

**Poster Presentation**

*Topics:* Catalysis for pollution control

*Keywords:* Graphene, Sulfamethoxazole, Photodegradation

**Application of N/S doping Graphene/TiO<sub>2</sub> on degradation of Sulfamethoxazole under visible irradiation**

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Titanium dioxide (TiO<sub>2</sub>) has emerged as a photocatalyst leader for environmental decontamination, however, the photocatalytic efficiency of TiO<sub>2</sub> is restricted under visible light irradiation because of the large intrinsic band gap (>3.2 eV) of TiO<sub>2</sub>. A variety of strategies have been adopted to enhance the photocatalytic efficiency of TiO<sub>2</sub>. The chemical modification of additional components in the TiO<sub>2</sub> structure is one of the most significant advancements [1-2]. In this study, a N/S doping rGraphene/TiO<sub>2</sub> 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/TiO<sub>2</sub> 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/TiO<sub>2</sub> photocatalysts were shifted to 420-466 nm and 417-454 nm, respectively. The degradation of SMX by N-doping rGO/TiO<sub>2</sub> and S-doping rGO/TiO<sub>2</sub> 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/TiO<sub>2</sub> 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/TiO<sub>2</sub> 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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Wednesday, 21/Aug/2019 3:52pm - 4:04pm

**Abstract ID: 773**

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**

**Ke-Fu Yao, Shuang-Qin Chen, Ji-Li Jia, Yao Tang, Yang Shao, Na Chen**

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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.

Wednesday, 21/Aug/2019 3:40pm - 3:52pm

**Abstract ID: 830**

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

**Ameemunisha Begum**

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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.

## **SYMPOSIUM 4: Functional Materials for Energy Storage and Conversion Devices (FESC)**

Thursday, 22/Aug/2019 3:06pm - 3:18pm

**Abstract ID: 122**

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**

**Bolong Huang**

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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 LiNbO<sub>3</sub> 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 VNb<sub>2</sub>O<sub>5</sub>, VLiNbO<sub>3</sub>, NbLi are also the energy conversion centers to non-radiative resonant energy transfer onto the activator center at the O<sub>i</sub> 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.

Thursday, 22/Aug/2019 1:30pm - 1:42pm

**Abstract ID: 140**

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

Oral Presentation

Topics: Hybrid cells for energy harvesting

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

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

**Muhammad S Khan<sup>1</sup>, Ashanul Ashanul Haque<sup>2</sup>, Rayya A Al-Balushi<sup>3</sup>, Idris J Al-Busaidi<sup>1</sup>**

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Poly-ynes and poly(metalla-ynes) 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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Thursday, 22/Aug/2019 8:00am - 8:12am

**Abstract ID: 167**

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 TiO<sub>2</sub> microsphere, Broadband harvesting, Near-infrared response

### **Enabling Low Energy Photons Harvesting for Efficient H<sub>2</sub> Production Employing PbS Nanocrystals Modified Anatase TiO<sub>2</sub> Microspheres**

**Tianyou Peng, Jinming Wang, Dong Liu, Chun Wu**

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Since the pioneering work on photosplitting water over TiO<sub>2</sub> electrode was reported in 1972,<sup>1</sup> photocatalytic H<sub>2</sub> 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.<sup>2,3</sup> Among which, TiO<sub>2</sub> 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%,<sup>2</sup> 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,<sup>4</sup> but its direct application in photocatalytic system for utilizing the low energy photons of solar spectrum is rare.<sup>5,6</sup> In this context, PbS nanocrystals (NCs) are used to modify anatase TiO<sub>2</sub> microspheres (AMS) to fabricate a novel PbS/AMS heterostructure enabling visible (Vis) and near-infrared (NIR) light harvesting for efficient H<sub>2</sub> 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 H<sub>2</sub> 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 H<sub>2</sub> production.

**Abstract ID: 169**

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

**Poster Presentation**

*Topics:* Nanogenerators and self-powered nanosystems

*Keywords:* micromotors, glucose, visible light, Cu<sub>2</sub>O, 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 applications<sup>1</sup>. Here, we report the fastest glucose-fuelled cuprous oxide@N doped carbon nanotube (Cu<sub>2</sub>O@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 Cu<sub>2</sub>O@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 H<sub>2</sub>O<sub>2</sub> fuels<sup>2</sup>. 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 water<sup>3</sup>. 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 Cu<sub>2</sub>O@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.

Wednesday, 21/Aug/2019 3:36pm - 3:48pm

**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

**Frederik Kunze<sup>1</sup>, Sophie Schnurre<sup>1</sup>, Tim Huelser<sup>1</sup>, Hartmut Wiggers<sup>2</sup>**

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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 (SiH<sub>4</sub>). 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 SiH<sub>4</sub> 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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Wednesday, 21/Aug/2019 1:36pm - 1:48pm

**Abstract ID: 193**

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**

**Giorgio Nava, Joseph Schwan, Lorenzo Mangolini**

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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 -C<sub>2</sub>H<sub>2</sub>- at 650 °C. After removing C<sub>2</sub>H<sub>2</sub>, 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<sup>-1</sup>, first cycle CE of 90% and stable cycling over 100 cycles.

Key Words: Silicon, Nano, Energy Storage

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Wednesday, 21/Aug/2019 2:12pm - 2:24pm

**Abstract ID: 196**

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, LiFePO<sub>4</sub>, Main Path Analysis

### An Overview of Research on Lithium Iron Phosphate Battery

**John S. Liu, Mei Hsiu-Ching Ho**

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This study aims to provide an overview on lithium iron phosphate (LiFePO<sub>4</sub>, 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 LiFePO<sub>4</sub> 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 LiFePO<sub>4</sub> nanoparticles.

Thursday, 22/Aug/2019 2:30pm - 2:42pm

**Abstract ID: 213**

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.

Wednesday, 21/Aug/2019 1:00pm - 1:12pm

**Abstract ID: 233**

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**

**Lihong Li**

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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<sub>0.96</sub>Sb<sub>0.04</sub>) O<sub>3</sub> were synthesized by the topological melting salt reaction with rod-like K<sub>2</sub> (Nb<sub>1-x</sub>Sb<sub>x</sub>)<sub>8</sub>O<sub>21</sub>. The molar ratio of sodium salt, (Li, Na, K) (Nb<sub>0.96</sub>Sb<sub>0.04</sub>) O<sub>3</sub> material was synthesized at approximating its quasi-isomorphic boundary. The ink of piezoelectric rod-like (Li, Na, K) (Nb<sub>0.96</sub>Sb<sub>0.04</sub>) O<sub>3</sub> 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<sub>0.96</sub>Sb<sub>0.04</sub>) O<sub>3</sub> 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: 241**

**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**

**Jun Shimizu, Shreeharsha Ramaswamy, Junho Choi**

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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.

Thursday, 22/Aug/2019 2:06pm - 2:18pm

**Abstract ID: 253**

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**

**Chengmei Jiang, Jianfeng Ping**

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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.

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

**Abstract ID: 281**

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**

**Fu-Ming Wang**

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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 1:42pm - 1:54pm

**Abstract ID: 282**

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

**Yungok Ihm<sup>1</sup>, Valentino Cooper<sup>2</sup>, Lukas Vlcek<sup>2</sup>, Pieremanuele Canepa<sup>3</sup>, Timo Thonhauser<sup>3</sup>, Ji Hoon Shim<sup>1</sup>, James Morris<sup>2</sup>**

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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.

Thursday, 22/Aug/2019 3:18pm - 3:30pm

**Abstract ID: 306**

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**

**Yu Ho, Holly Kwok<sup>1</sup>, Yifei Wang<sup>1</sup>, Yingguang Zhang<sup>1</sup>, Huimin Zhang<sup>2</sup>, Yiu Cheong, Dennis Leung<sup>1</sup>**

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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.

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

**Abstract ID: 325**

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

Oral Presentation

Topics: Electrochemical Supercapacitors

Keywords: supercapacitors, wearable electronics, inkjet printing, Ni<sub>2</sub>CO<sub>3</sub>

### **Inkjet Printing-Assisted Growth of Ni<sub>2</sub>CO<sub>3</sub> Nano-Rods over Fabric Substrates for Flexible and Wearable Supercapacitor Applications**

**Poonam Sundriyal, Shantanu Bhattacharya**

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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 Ni<sub>2</sub>CO<sub>3</sub> 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 Ni<sub>2</sub>CO<sub>3</sub> nanorods// AC exhibits excellent electrochemical performance upto 1.6 V in the LiClO<sub>4</sub> electrolyte. Figure 1 shows the schematic of the device assembly and FESEM image of the grown nanorods of Ni<sub>2</sub>CO<sub>3</sub> 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 1:24pm - 1:36pm

**Abstract ID: 358**

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**

**Arun Thirumurugan<sup>1</sup>, Ali Akbari-Fakhranadi<sup>1</sup>, Prabakaran K<sup>2</sup>**

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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 Fe<sub>3</sub>O<sub>4</sub> and Fe<sub>2</sub>O<sub>3</sub> 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 Fe<sub>3</sub>O<sub>4</sub> 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 2:54pm - 3:06pm

**Abstract ID: 387**

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

**LEONARDO VIVAS<sup>1</sup>, ADRIAN JARA CORNEJO<sup>2</sup>, DINESH PRATAP SINGH<sup>3</sup>**

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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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**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**

**Jun Woo Jeon<sup>1,2</sup>, Dong-Min Kim<sup>2</sup>, Minsu Kim<sup>1</sup>, Yong Seok Kim<sup>1</sup>, Jong-Chan Lee<sup>2</sup>, Kyu Tae Lee<sup>2</sup>, Byoung Gak Kim<sup>1</sup>**

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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<sup>1, 2</sup> and sodium sulfur batteries<sup>3, 4</sup>. 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.<sup>5, 6</sup> Aside from these benefits, both sodium (Na) and sulfur (S) possesses a high theoretical specific capacity of 1166 mA h g<sup>-1</sup> and 1675 mA h g<sup>-1</sup>, respectively.<sup>7</sup> Especially, room Temperature Na-S (RT Na-S) batteries have been considered as a reasonable option due to safety problems and low operating cost. <sup>8</sup> However, low electrical conductivity of sulfur and polysulfide dissolution still exist so as to fully exploit the potential of these Na-S batteries.<sup>1, 6</sup> Especially, the soluble long chain sodium polysulfide (Na<sub>2</sub>S<sub>x</sub>, 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.<sup>9</sup> 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 (Na<sub>2</sub>S<sub>x</sub>, 4 ≤ x ≤ 8) was fundamentally inhibited. The strategy lead to the long cycling stability for 100 cycles with capacity of 400 mA h gs<sup>-1</sup> 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: 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**

**Byoung Gak Kim, Jun Woo Jeon, Jae Hee Han, Minsu Kim, Yong Seok Kim, Tae-Ho Kim**

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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.<sup>1, 2</sup> 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.<sup>3, 4</sup> 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.<sup>5</sup> 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 ( $150\text{ S cm}^{-1}$ ), high specific capacitances (363, 261, and  $200\text{ F g}^{-1}$  in three-, two-electrode aqueous systems, and two-electrode organic systems, respectively) at  $1\text{ A g}^{-1}$ , and exceptional specific energy of  $43.2\text{ Wh kg}^{-1}$  at a specific power of  $1.25\text{ kW kg}^{-1}$ , 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 1:54pm - 2:06pm

**Abstract ID: 439**

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**

**Hiroataka Fujimori<sup>1</sup>, Ippei Kawanishi<sup>1</sup>, Nobuhiro Matsushita<sup>2</sup>**

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According to our diffraction study described in the presentation (1), photocatalytic water-splitting performance on Sr<sub>2</sub>Ta<sub>2</sub>O<sub>7</sub> 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 TaO<sub>6</sub>/NbO<sub>6</sub> octahedra. For Sr<sub>2</sub>Nb<sub>2</sub>O<sub>7</sub>, one of the related compounds of Sr<sub>2</sub>Ta<sub>2</sub>O<sub>7</sub>, the strength of the internal Nb-O bonds in NbO<sub>6</sub> octahedra was as weak as the external bonds. The weak Nb-O chemical bonds induce the large distortions of the NbO<sub>6</sub> octahedra and the static displacements of Nb ions from the gravity center of six O ions in the NbO<sub>6</sub> octahedra. They are as crucial as the static NbO<sub>6</sub> 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 Sr<sub>2</sub>Ta<sub>2</sub>O<sub>7</sub> for Sr, the strength of the internal Ta-O bonds in TaO<sub>6</sub> 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 TaO<sub>6</sub> 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 Ta<sub>5d</sub>-t<sub>2g</sub> and O<sub>2p</sub> orbitals composing the lower part of the conduction band.

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

**Abstract ID: 440**

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

**Ippei Kawanishi<sup>1</sup>, Hiroataka Fujimori<sup>1</sup>, Masatomo Yashima<sup>2</sup>**

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Sr<sub>2</sub>Ta<sub>2</sub>O<sub>7</sub> with NiOx 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 Sr<sub>2</sub>Ta<sub>2</sub>O<sub>7</sub>, 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 Sr<sub>2</sub>Ta<sub>2</sub>O<sub>7</sub>, such as changes in the angle of the TaO<sub>6</sub> octahedral tilts and/or in the degree of distortions of TaO<sub>6</sub> 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 Sr<sub>2</sub>Ta<sub>2</sub>O<sub>7</sub> increases the TaO<sub>6</sub> octahedral tilts and the distortions in TaO<sub>6</sub> octahedra, which induce dipole moments in TaO<sub>6</sub> octahedra and the spontaneous polarization. The electronic field in whole crystal of Sr<sub>2</sub>Ta<sub>2</sub>O<sub>7</sub> (the spontaneous polarization) and/or the local electric field around Ta ions (the dipole moments) seemingly enhance the photocatalytic activity of NiOx-supported Sr<sub>2</sub>Ta<sub>2</sub>O<sub>7</sub> 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 TaO<sub>6</sub> 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 Ta5d-t<sub>2g</sub> and O2p 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°.

Wednesday, 21/Aug/2019 2:48pm - 3:00pm

**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.

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

**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**

**Nicholas Musyoka, Jianwei Ren, Henrietta Langmi, Mkhulu Mathe**

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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.

Thursday, 22/Aug/2019 8:48am - 9:00am

**Abstract ID: 468**

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**

**Bilge Saruhan-Brings<sup>1</sup>, Masud Rana<sup>1</sup>, Jan Petersen<sup>2</sup>, Sebastian Geier<sup>2</sup>**

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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 LiClO<sub>4</sub> 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: 473**

**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 $\text{Ge}_{1-x}\text{Bi}_x\text{Te}$ crystals**

**Yang-Yuan Chen<sup>1</sup>, Pai-Chun Wei<sup>1,2</sup>, Cheng-Lung Chen<sup>1</sup>**

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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  $\text{Ge}_{1-x}\text{Bi}_x\text{Te}$  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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**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**

**Dongseob Kim<sup>1</sup>, Sangmin Lee<sup>2</sup>**

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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.

Thursday, 22/Aug/2019 9:12am - 9:24am

**Abstract ID: 494**

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**

**Yaping Zhao, Huijun Tan**

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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.

Wednesday, 21/Aug/2019 2:24pm - 2:36pm

**Abstract ID: 505**

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

Plenary

*Topics:* Artificial photosynthesis

*Keywords:* CO2 reduction, Graphene, Nano, photoconversion

### **Photoconversion of CO<sub>2</sub>: Controllable Transition from C1 to C2 Products**

**SU-IL IN**

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Photocatalytic reduction of CO<sub>2</sub> 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 CO<sub>2</sub> 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, C<sub>2</sub>H<sub>6</sub>, 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 CH<sub>4</sub> to C<sub>2</sub>H<sub>6</sub>. We find the switch from C1 to C2 products is dependent upon upward band bending at the reduced blue-titania/graphene interface.

**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**

**Tai-Ho Yu, Tung-Che Lu**

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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.

**Tuesday, 20/Aug/2019 4:12pm - 4:24pm**

**Abstract ID: 612**

**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**

**Ramakrishna Podila, Chengxin Wang, Bingan Lu, Apparao Rao**

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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 ( $\text{AlCl}_4^-$ ) 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: 621**

**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**

**Yong Ren, Jing Wang**

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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: 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:* NaNbO<sub>3</sub>, 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 NaNbO<sub>3</sub> Type-II Heterostructures: A Promising Photocatalyst For H<sub>2</sub> Production**

**Francis Opoku<sup>1</sup>, Krishna Kuben Govender<sup>2</sup>, Cornelia Gertina Catharina Elizabeth van Sittert<sup>3</sup>, Penny Poomani Govender<sup>4</sup>**

<sup>1</sup>University of Johannesburg, South Africa; <sup>2</sup>Center for High Performance Computing, South Africa; <sup>3</sup>North-West University, South Africa; <sup>4</sup>University of Johannesburg, South Africa; [ofrancis2010@gmail.com](mailto:ofrancis2010@gmail.com)

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 NaNbO<sub>3</sub> 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 NaNbO<sub>3</sub> (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, NaNbO<sub>3</sub> is doped with V<sup>5+</sup>, which is then coupled with a GO sheet. The suitable type-II heterojunction structure between NaNbO<sub>3</sub> (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 NaNbO<sub>3</sub>. The GO/V-doped NaNbO<sub>3</sub> (100) heterostructure is a direct band gap semiconductor with a smaller effective mass compare with the pure NaNbO<sub>3</sub>, which shows that the heterostructure has a higher charge carrier mobility. Thus, the resulting bifunctional GO/V-doped NaNbO<sub>3</sub> (100) heterostructure is endowed with a suitable band alignment, narrow band gap, negatively charged O atoms on the NaNbO<sub>3</sub> (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**

**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:* SrTiO<sub>3</sub>; environmental and energy crises; type-II band alignment; environmental contamination; hybrid DFT

**First-Principles Study of Cubic SrTiO<sub>3</sub> with Perovskite-Type Materials MTaO<sub>3</sub> (M = Na, K) for Environmental Remediation**

**Penny Poomani Govender<sup>1</sup>, Francis Opoku<sup>2</sup>, Krishna Kuben Govender<sup>3</sup>, Cornelia Gertina Catharina Elizabeth van Sittert<sup>4</sup>**

<sup>1</sup>University of Johannesburg, South Africa; <sup>2</sup>University of Johannesburg, South Africa; <sup>3</sup>Center for High Performance Computing, South Africa; <sup>4</sup>North-West University, South Africa; [pennyg@uj.ac.za](mailto:pennyg@uj.ac.za)

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 MTaO<sub>3</sub>/SrTiO<sub>3</sub>(010) (M = Na, K) heterostructures photocatalyst material for environmental remediation. In this study, the stability, electronic and optical properties of coupled MTaO<sub>3</sub> and SrTiO<sub>3</sub> were systematically studied using the hybrid HSE06 method. The MTaO<sub>3</sub>/SrTiO<sub>3</sub>(010) heterostructures show high photocatalytic activity under visible light irradiation with good stability and reduced bandgap compared to the bulk SrTiO<sub>3</sub>. 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 MTaO<sub>3</sub>/SrTiO<sub>3</sub>(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 MTaO<sub>3</sub>/SrTiO<sub>3</sub>(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 SrTiO<sub>3</sub> to the Ta 5d state of MTaO<sub>3</sub>. In summary, this study shows a key role of SrTiO<sub>3</sub> as an electron donor to enhance the optical properties and stability of MTaO<sub>3</sub>/SrTiO<sub>3</sub>(010) heterostructures.

Wednesday, 21/Aug/2019 6:28pm - 6:40pm

**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**

**Phumlani Msomi<sup>1</sup>, Vhahangwele Mudzunga<sup>1</sup>, Rudzani Sigwadi<sup>2</sup>, Patrick Nonjola<sup>3</sup>**

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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, TiO<sub>2</sub>, 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.

Thursday, 22/Aug/2019 8:24am - 8:36am

**Abstract ID: 686**

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**

**Nasim Anjum, Caiwei Shen**

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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/cm<sup>2</sup>, 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.

Thursday, 22/Aug/2019 10:00am - 10:12am

**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 BaTiO<sub>3</sub> piezoelectric composites**

**Paula Ferreira, Dayana Sierra, Cláudia Nunes, Paula Vilarinho**

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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 BaTiO<sub>3</sub> 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 9:00am - 9:12am

**Abstract ID: 726**

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**

**Zhaohuai Li, Qiu He, Xu Xu, Liqiang Mai**

Wuhan University of Technology, China, People's Republic of; [xuxu@whut.edu.cn](mailto:xuxu@whut.edu.cn)

Lithium-sulfur (Li-S) batteries have attracted remarkable attention due to their high theoretical capacity of 1675 mAh g<sup>-1</sup>, 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<sup>-1</sup> and the capacity remains 1267 mAh g<sup>-1</sup> after 100 cycles at 0.5 C. Even at 5 C, a capacity of 676 mAh g<sup>-1</sup> is reached. With a high sulfur loading of 9.6 mg cm<sup>-2</sup>, 3DNG cathode achieves an ultra-high areal capacity of 12.0 mAh cm<sup>-2</sup> at the high current density of 8.03 mA cm<sup>-2</sup>. This proposal unique structure gives the bright prospect that high energy density and high power density can be achieved simultaneously for Li-S battery.

Thursday, 22/Aug/2019 8:36am - 8:48am

**Abstract ID: 748**

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

**Oskar Paris<sup>1</sup>, Christian Koczwara<sup>1</sup>, Christian Prehal<sup>2</sup>**

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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.

#### References

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3. C. Prehal, C. Koczwara, H. Amenitsch, V. Presser, O. Paris, *Nature Communications* 9 (2018) 4145.

Wednesday, 21/Aug/2019 1:48pm - 2:00pm

**Abstract ID: 749**

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**

**Zbigniew Stempień<sup>1</sup>, Mohammad Khalid<sup>2</sup>, Marek Kozicki<sup>1</sup>**

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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/H<sub>3</sub>PO<sub>4</sub> 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/cm<sup>2</sup> and 113 to 553 F/g in dependence of scan rate.

**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**

**Jang Myoun Ko, Mwemezi Manasi**

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Hydroxy terminated poly(dimethylsiloxane) (PDMS-HT) is used as an electrolyte additive in electrolyte systems containing 1 M LiPF<sub>6</sub> 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<sup>+</sup> 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.

Thursday, 22/Aug/2019 2:18pm - 2:30pm

**Abstract ID: 818**

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**

**Sankha Mukherjee, Chandraveer Singh**

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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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[2] Mukherjee, S., Song, J., & Vengallatore, S. (2016). Atomistic simulations of material damping in amorphous silicon nanoresonators. *Modelling and Simulation in Materials Science and Engineering*, 24(5), 055015.

Wednesday, 21/Aug/2019 1:12pm - 1:24pm

**Abstract ID: 821**

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 (ZrO<sub>2</sub>) NPs, piezoelectricity and piezoelectric nanogenerator.

**Use of ZrO<sub>2</sub> Stimulated PVDF HFP Composite Flexible Thin Film in developing High Performance Piezoelectric Nanogenerator and Transparent Single Electrode Triboelectric Nanogenerator**

**Sukhen Das<sup>1</sup>, Minarul Shaikh<sup>2</sup>, Nur Amin Hoque<sup>1</sup>, Prosenjit Biswas<sup>1</sup>, Pradip Thakur<sup>3</sup>**

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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 (ZrO<sub>2</sub>) manipulated electroactive poly vinylidene fluoride–hexafluoropropylene (PVDF HFP) nanocomposite films, have been observed. In ZrO<sub>2</sub>/PVDF HFP, ZrO<sub>2</sub> 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<sub>oc</sub>~120 Volt) and short circuit current (I<sub>sc</sub> ~1.95 μA) under periodic finger imparting with high power density ~ 7091 μWcm<sup>-3</sup>. 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.

Thursday, 22/Aug/2019 2:42pm - 2:54pm

**Abstract ID: 823**

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**

**Ruma Basu<sup>1</sup>, Nur Amin Hoqu<sup>2</sup>, Prosenjit Biswas<sup>2</sup>, Sukhen Das<sup>2</sup>, Pradip Thakur<sup>3</sup>**

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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  $\beta$  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  $\beta$  phase, resulting in the radical increase in dielectric constant ( $\sim 40.6$ ) 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  $\sim 83$  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 ( $\sim 6$  V) has been produced by mere figure touch.

*Keywords:* Piezoelectric nanogenerator, PVDF/CuS NRs, Dielectric constant

Wednesday, 21/Aug/2019 3:12pm - 3:24pm

**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

**Manu Saji Samuel, Chirag Mevada, Mausumi Mukhopadhyay**

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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 H<sub>2</sub>SO<sub>4</sub>:HNO<sub>3</sub> (3:1 v/v) followed by NH<sub>4</sub>OH 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<sup>-2</sup> at 1.5 mA cm<sup>-2</sup> in 1 M H<sub>2</sub>SO<sub>4</sub> 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: 833**

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

**Poster Presentation**

*Topics:* Solar Cells

*Keywords:* Perovskite solar cells, SnO<sub>2</sub> quantum dots, electron transport layer, air-processed PSCs.

### **Air-processed perovskite solar cells made with SnO<sub>2</sub> quantum dots**

**P.-J. Mo<sup>1</sup>, James Wang<sup>2</sup>, Hong Paul Wang<sup>1</sup>**

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SnO<sub>2</sub> 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 TiO<sub>2</sub>. Therefore, large-scale perovskite solar cells (PSCs) incorporating SnO<sub>2</sub> as the ETL may have a higher stability. SnCl<sub>2</sub>•2H<sub>2</sub>O in DI water can be self-evolved into SnO<sub>2</sub> quantum dots through the hydrolysis-oxidation process with urea as an additive to accelerate the reaction. The SnO<sub>2</sub> layer can be easily fitted in PSCs by spin coating. The power conversion efficiency (PCE) of the SnO<sub>2</sub>-based PSC is as high as 12.5% in the reverse scan with the configuration of FTO/SnO<sub>2</sub>/perovskite/CuPc/carbon paste. The active area of the PSCs was 0.1 cm<sup>2</sup> 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**

**M.-X. Zhuang<sup>1</sup>, P.-J. Mo<sup>1</sup>, James Wang<sup>2</sup>, Y.-L. Wei<sup>3</sup>, Hong Paul Wang<sup>1</sup>**

<sup>1</sup>Department of Environmental Engineering, National Cheng Kung University, Tainan 70101, Taiwan; <sup>2</sup>Department of Nanoengineering, University of California, San Diego, CA 92037, USA; <sup>3</sup>Department of Environmental Science and Engineering, Tunghai University, Taichung 40704, Taiwan; [yulin@mail.thu.edu.tw](mailto:yulin@mail.thu.edu.tw)

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/CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>/porous TiO<sub>2</sub>/compact TiO<sub>2</sub>/FTO, fabricated under a humid atmosphere of 50% RH and demonstrated a power conversion efficiency of 6.72%.

**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 WSe<sub>2</sub> density functional theory calculation

**DFT Study of Skutterudite CoSb<sub>3</sub> and In<sub>0.2</sub>Co<sub>4</sub>Sb<sub>12</sub> Thermoelectric Heterostructures with 2D-WSe<sub>2</sub>**

**Ephraim Muriithi Kiariri<sup>1</sup>, Krishna Kuben Govender<sup>2</sup>, Messai Adenew Mamo<sup>1</sup>, Penny Poomani Govender<sup>1</sup>**

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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  $S$ ,  $\sigma$ ,  $T$ ,  $k_e$  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 WSe<sub>2</sub> transition-metal dichalcogenides have been used for novel electronic devices. However, its influence on the electronic and optical properties of thermoelectric Skutterudite CoSb<sub>3</sub> and In<sub>0.2</sub>Co<sub>4</sub>Sb<sub>12</sub> is unknown. Despite the increased potential of energy conversion obtained by doping CoSb<sub>3</sub> with indium, further theoretical study is necessary to understand the origin of this enhancement. Heterostructures of hybrid WSe<sub>2</sub>/CoSb<sub>3</sub> and WSe<sub>2</sub>/In<sub>0.2</sub>Co<sub>4</sub>Sb<sub>12</sub> 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 CoSb<sub>3</sub> has a bandgap of 0.456 eV, and In<sub>0.2</sub>Co<sub>4</sub>Sb<sub>12</sub> has a zero bandgap, while the calculated bandgap for WSe<sub>2</sub> 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 2:36pm - 2:48pm

**Abstract ID: 841**

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**

**Lin Wang<sup>1</sup>, Samuel Welborn<sup>1</sup>, Eric Detsi<sup>1,2</sup>**

<sup>1</sup>Department of Materials Science & Engineering, University of Pennsylvania, Philadelphia PA 19104-6272, USA; <sup>2</sup>Vagelos Institute for Energy Science and Technology (VIEST), Philadelphia, PA 19104, USA; [wanglin1@seas.upenn.edu](mailto:wanglin1@seas.upenn.edu)

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 30-40°C. Operando X-ray scattering techniques were used to demonstrate this self-healing property in real-time during magnesiation and demagnesiation.

**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**

**Yuan Jiang, Xumin Gao, Jialei Yuan, Yan Jiang, Zheng Shi, Linning Wang, Ruixue Jin, yongjin wang**

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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  $\lambda$  (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**

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**

**Jintao Fu<sup>1</sup>, John Corsi<sup>1,2</sup>, Manni Li<sup>1,3</sup>, Eric Detsi<sup>1,2</sup>**

<sup>1</sup>Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, USA; <sup>2</sup>Vagelos Institute for Energy Science and Technology (VIEST), Philadelphia, USA;

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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  $\text{NaTMO}_2$  (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.

Wednesday, 21/Aug/2019 3:00pm - 3:12pm

**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**

**John Corsi<sup>1,2</sup>, Eric Stach<sup>1,2</sup>, Eric Detsi<sup>1,2</sup>**

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High-capacity alloy-type lithium-ion battery anodes can undergo large volume changes (~300%) during lithiation.<sup>1</sup> 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.<sup>1</sup> 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.<sup>2</sup> 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 “nanobattery<sup>3</sup>” 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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Wednesday, 21/Aug/2019 2:00pm - 2:12pm

**Abstract ID: 862**

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

**Samuel S. Welborn<sup>1</sup>, John S. Corsi<sup>1</sup>, Eric Detsi<sup>1,2</sup>**

<sup>1</sup>University of Pennsylvania, Philadelphia, PA, USA.; <sup>2</sup>Vagelos Institute for Energy Science and Technology (VIEST), Philadelphia, PA, USA.; [swelborn@seas.upenn.edu](mailto:swelborn@seas.upenn.edu)

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.<sup>1,2</sup> 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,  $\epsilon$  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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## **SYMPOSIUM 5: Functional Low dimensional, Nano and 2D materials (FLNM)**

Thursday, 22/Aug/2019 2:42pm - 2:54pm

**Abstract ID: 120**

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**

**Petr Kovaricek**

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

**Abstract ID: 165**

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**

**Justin Sambur**

Colorado State University, United States of America; [jsambur@colostate.edu](mailto:jsambur@colostate.edu)

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.

**Tuesday, 20/Aug/2019 3:48pm - 4:00pm**

**Abstract ID: 168**

**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**

**Surojit Gupta**

University of North Dakota, United States of America; [surojit.gupta@engr.und.edu](mailto:surojit.gupta@engr.und.edu)

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.

**Thursday, 22/Aug/2019 9:12am - 9:24am**

**Abstract ID: 175**

**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**

**David Michael Black<sup>1</sup>, Priscilla Lopez<sup>1</sup>, Elizabeth Orr<sup>2</sup>, Humberto Herman Lara<sup>3</sup>, Marcos Miguel Alvarez<sup>2</sup>, Glen Baghdesarian<sup>2</sup>, Jose Luis Lopez Ribot<sup>3</sup>, Robert Loyd Whetten<sup>3</sup>, Christine Moon<sup>2</sup>**

<sup>1</sup>Department of Physics & Astronomy, University of Texas, San Antonio, Texas 78249;

<sup>2</sup>Department of Chemistry Los Angeles City College, United States of America; <sup>3</sup>Department of Biology and South Texas Center for Emerging Infectious Diseases, University of Texas, San Antonio, Texas 78249; [humberto.laravillegas@utsa.edu](mailto:humberto.laravillegas@utsa.edu)

In 1982, Dr Jim Hainfeld demonstrated that a gold-cluster (Au<sub>11</sub>(PPh<sub>3</sub>)<sub>7</sub>I<sub>3</sub>) could be obtained in a water-soluble form and modified by conjugation of the Ph\*<sup>-</sup>groups to biomolecular groups.<sup>1,2</sup> This molecule has enhanced stability because its 8 "free" electrons occupy a closed-shell S<sub>2</sub>P<sub>6</sub> configuration of globular 'super-atomic' orbitals.<sup>3</sup> 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 (Ag<sub>29</sub>) cluster and 12 lipoic acid ligands.<sup>4</sup> 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 Ag<sub>29</sub> lipocate 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

**References**

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Thursday, 22/Aug/2019 11:04am - 11:16am

**Abstract ID: 177**

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**

**Jubaraj Bikash Baruah**

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Emission Properties of Organic Fluorescent Molecules in Solid and Solution

Jubaraj B. Baruah

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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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Thursday, 22/Aug/2019 10:40am - 10:52am

**Abstract ID: 207**

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**

**Xuecheng Yu, Mohamed Kilani, Evan Schaefer, Long Luo, Guangzhao Mao**

Wayne State University, United States of America; [guangzhao.mao@wayne.edu](mailto:guangzhao.mao@wayne.edu)

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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Thursday, 22/Aug/2019 2:30pm - 2:42pm

**Abstract ID: 229**

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**

**Melinda Jue, Chiatai Chen, Steven Buchsbaum, Eric Meshot, Sei Jin Park, Kuang Jen Wu, Francesco Fornasiero**

Lawrence Livermore National Laboratory, United States of America; [jue6@llnl.gov](mailto:jue6@llnl.gov)

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  $2 \times 10^{12}$  tubes/cm<sup>2</sup>) 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  $4 \times 10^{-5}$  mol/m<sup>2</sup> 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.

Thursday, 22/Aug/2019 3:06pm - 3:18pm

**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**

**Steven Buchsbaum, Melinda Jue, April Marie Sawvel, Chiatai Chen, Eric Meshot, Sei Jin Park, Kaung Jen Wu, Edmond Y. Lau, Tuan Anh Pham, Francesco Fornasiero**

Lawrence Livermore National Laboratory, United States of America; [buchsbaum1@llnl.gov](mailto:buchsbaum1@llnl.gov)

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.

Thursday, 22/Aug/2019 11:40am - 11:52am

**Abstract ID: 251**

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 MoS<sub>2</sub> nanosheets, nanocomposite, stretchable strain sensor, triboelectric nanogenerator.

**Highly Conductive Composite Film of Silver Nanowires Network “Nanosoldered”  
by Metallic MoS<sub>2</sub> Nanosheets for Stretchable Strain Sensor and Self-powered  
Triboelectric Nanogenerator**

**Lingyi Lan, Jianfeng Ping, Yibin Ying**

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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 MoS<sub>2</sub> nanosheets. This mixed-dimensional structure (1D–2D) composite film with excellent properties combines the flexibility of 2D MoS<sub>2</sub> nanosheets with conductive and stretchable 1D AgNWs network. In addition, the large surface area, mechanical flexibility, and strong bonding with AgNWs enable the metallic MoS<sub>2</sub> nanosheets to wrap around and nanosolder the AgNWs junctions, which could significantly reduce the resistance of the composite. Results show that AgNWs-MoS<sub>2</sub> 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-MoS<sub>2</sub>/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.

Thursday, 22/Aug/2019 3:30pm - 3:42pm

**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**

**Ankit Soni, Komal Mulchandani, Krushna R Mavani**

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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 (PO<sub>2</sub>) 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 PO<sub>2</sub> in step-2. The prepared nanostructures were studied for the parametric effects on growth, porosity and optical properties. For series-1, N<sub>2</sub> adsorption-desorption isotherms and the surface analysis reveals the porous nature of nanostructures grown with varied PO<sub>2</sub>. At PO<sub>2</sub> of 7.5 Pa, the surface morphology and growth of ZnO nanostructure is very different (Fig. a) and it changes gradually with higher PO<sub>2</sub> (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.

Thursday, 22/Aug/2019 2:06pm - 2:18pm

**Abstract ID: 318**

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**

**Mukesh Kumar Thakur, Akash Gupta, Surojit Chattopadhyay**

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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 SiO<sub>2</sub>@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 x10<sup>3</sup> AW<sup>-1</sup>, 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 9:24am - 9:36am

**Abstract ID: 331**

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**

**Sandeep Singh**

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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.

Thursday, 22/Aug/2019 10:00am - 10:12am

**Abstract ID: 335**

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**

**Qiming Qiu, Yixian Wang, Huayun Chen**

Zhejiang University, China, People's Republic of; [qimingqiu@zju.edu.cn](mailto:qimingqiu@zju.edu.cn)

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 12:04pm - 12:16pm

**Abstract ID: 352**

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**

**AZAM ALI**

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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.

**Abstract ID: 357**

**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**

**Victor Genchev Ivanov<sup>1</sup>, Eric Faulques<sup>2</sup>, Jeremy Sloan<sup>3</sup>, Nataliya Kalashnyk<sup>4</sup>**

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<sup>3</sup>Department of Physics, University of Warwick, United Kingdom; <sup>4</sup>GeePs, CNRS UMR 8507 – CentraleSupélec – UPSud – UPMC, France; [vgi@phys.uni-sofia.bg](mailto:vgi@phys.uni-sofia.bg)

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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**Abstract ID: 361**

**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**

**Piboonwan Insiti<sup>1</sup>, Attasith Parnsubsakul<sup>1,2</sup>, Umphan Ngoensawat<sup>1</sup>, Chaweewan Sapcharoenkun<sup>3</sup>, Sanong Ekgasit<sup>1,2</sup>**

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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  $\mu\text{m}$  thickness) was solvent casted on a polydimethylsiloxane (PDMS) film from a 2- $\mu\text{L}$  drop of BNC colloid before drying at 100  $^{\circ}\text{C}$  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- $\mu\text{L}$  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  $\mu\text{g}$  of gold metal was deposited on the BNC film.

Thursday, 22/Aug/2019 8:36am - 8:48am

**Abstract ID: 366**

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

**Xin Zhao<sup>1,2</sup>, Dimitrios Papageorgiou<sup>1</sup>, Wen Zhao<sup>3,4</sup>, Feng Ding<sup>3,4</sup>, Robert Young<sup>1,3</sup>**

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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.

Thursday, 22/Aug/2019 8:48am - 9:00am

**Abstract ID: 371**

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**

**Sam-Soo Kim, Sung-Eun Park, Gyuseok Choi, Yoonkap Kim**

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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.

Thursday, 22/Aug/2019 11:16am - 11:28am

**Abstract ID: 388**

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**

**Eric Faulques<sup>1</sup>, Jeremy Sloan<sup>2</sup>, Victor Genchev Ivanov<sup>3</sup>, Stéphane Cordier<sup>4</sup>, Yann Molard<sup>4</sup>, Karine Costuas<sup>4</sup>, Jean-Luc Duvail<sup>1</sup>, Florian Massuyeau<sup>1</sup>, Nataliya Kalashnyk<sup>5</sup>**

<sup>1</sup>CNRS, IMN, University of Nantes, France; <sup>2</sup>University of Warwick, United Kingdom; <sup>3</sup>Sofia University, Bulgaria; <sup>4</sup>Institut des Sciences Chimiques de Rennes, University of Rennes, France; <sup>5</sup>GeePs, CNRS UMR 8507 – CentraleSupélec – UPSud – UPMC, Gif sur Yvette, France;

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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.

Thursday, 22/Aug/2019 3:18pm - 3:30pm

**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**

**Daša Paulenová, Ján Marták, Štefan Schlosser**

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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% tetradecyltriethylphosphonium 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.

Thursday, 22/Aug/2019 12:16pm - 12:28pm

**Abstract ID: 432**

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**

**Mark Wayne Lee Jr., Teng-Wei Wang, Dronareddy Madugula, Madison Clark**

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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  $[B_{12}H_{12}]^{2-}$ , as well as the ten-vertex closo-decaborate  $[B_{10}H_{10}]^{2-}$ . 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.

Thursday, 22/Aug/2019 1:42pm - 1:54pm

**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**

**Hongliang Hao, Shuai Wang, Huanhuan Li, Qingmeng Wu, Yingcui Fang**

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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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Thursday, 22/Aug/2019 10:36am - 10:48am

**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

**Jing Wang, Mustafa EGINLIGIL**

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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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Thursday, 22/Aug/2019 9:00am - 9:12am

**Abstract ID: 467**

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**

**Ali Almaqwashi<sup>1</sup>, Aly Fouda<sup>1,2</sup>, El Shazly Duraia<sup>2</sup>**

<sup>1</sup>KAU, Saudi Arabia; <sup>2</sup>Suez Canal University, Egypt; [aalmaqwashi@kau.edu.sa](mailto:aalmaqwashi@kau.edu.sa)

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 9:48am - 10:00am

**Abstract ID: 477**

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**

**Dan Tan<sup>1,2</sup>, Morten Willatzen<sup>1,2</sup>**

<sup>1</sup>Beijing Institute of Nanoenergy and Nanosystem, China, People's Republic of; <sup>2</sup>School of Nanoscience and Technology, University of Chinese Academy of Sciences, Beijing 100049, P. R. China; [tandan@binn.cas.cn](mailto:tandan@binn.cas.cn)

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.

Thursday, 22/Aug/2019 2:18pm - 2:30pm

**Abstract ID: 482**

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.

Thursday, 22/Aug/2019 3:42pm - 3:54pm

**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

**Yanlin Song**

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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 ( $12\pm 3$  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 electronical 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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**Tuesday, 20/Aug/2019 9:30am - 10:00am**

**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  $\pi$ -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.<sup>1</sup> 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 grapheme.<sup>2,3</sup> 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.<sup>4-6</sup> 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.<sup>7</sup>

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Thursday, 22/Aug/2019 11:52am - 12:04pm

**Abstract ID: 511**

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**

**Moh Amer**

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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 MoS<sub>2</sub> nanosheets using Raman spectroscopy [1]. These MoS<sub>2</sub> nanosheets exhibit anomalous particle formation on the surface after laser irradiation. Our results demonstrate monolayer MoS<sub>2</sub> exhibit different behavior than few layers MoS<sub>2</sub>, 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 HfSe<sub>2</sub> material. This material is known to be n-type. However, our results show HfSe<sub>2</sub> 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 HfSe<sub>2</sub>. I will finally conclude with future outlook of layered 2D materials in photonic and electronic applications.

Thursday, 22/Aug/2019 11:28am - 11:40am

**Abstract ID: 518**

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

**Wojciech Kempniński<sup>1</sup>, Mateusz Kempniński<sup>2</sup>**

<sup>1</sup>Institute of Molecular Physics, Polish Academy of Sciences, Poland; <sup>2</sup>Faculty of Physics and NanoBioMedical Centre Adam Mickiewicz University, Poland; [wojkem@ifmpan.poznan.pl](mailto:wojkem@ifmpan.poznan.pl)

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: 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**

**Yue Shen<sup>1</sup>, Yanxia Sun<sup>1</sup>, Chunxi Hai<sup>1</sup>, Yuan Zhou<sup>1</sup>, Yi Zhang<sup>2</sup>**

<sup>1</sup>Key Laboratory of Salt Lake Resources Chemistry of Qinghai Province, Qinghai Institute of Salt Lakes, Chinese Academy of Sciences, Xining, Qinghai 810008, China; <sup>2</sup>Key Laboratory of Interfacial Physics and Technology of Chinese Academy of Sciences, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 201800, China; [shenyue@isl.ac.cn](mailto:shenyue@isl.ac.cn)

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.

**Abstract ID: 558**

**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**

**Xiaolu Zhu, Yingda Wang, Wenjie Zhao, Chunwang Xu**

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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- $\mu\text{m}$  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 ( $\text{Cu}^{2+}$  and  $\text{Pd}^{2+}$ ) 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.

Thursday, 22/Aug/2019 2:54pm - 3:06pm

**Abstract ID: 607**

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, MoTe<sub>2</sub>, Ionic Liquid, Raman

### **Reversible 2H to 1T' Phase Change in Monolayer to Bulk MoTe<sub>2</sub> by Ionic Liquid Gating**

**Dante Zakhidov, Daniel Rehn, Evan Reed, Alberto Salleo**

Stanford University, United States of America; [zakhidov@stanford.edu](mailto:zakhidov@stanford.edu)

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.<sup>1</sup> Out of the TMDs, MoTe<sub>2</sub> is attractive for electronic applications because it has the lowest energy difference between the semiconducting (2H) and semi-metallic (1T') phases which makes the MoTe<sub>2</sub> phase change feasible by electrostatic doping.<sup>2,3</sup> Here we report reversible, electrostatic phase change of MoTe<sub>2</sub> in all thicknesses of MoTe<sub>2</sub>, 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 MoTe<sub>2</sub> 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' phase<sup>4</sup>, potentially aiding the phase change process. Our work demonstrates the feasibility of MoTe<sub>2</sub> 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 12:28pm - 12:40pm

**Abstract ID: 608**

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

### Self-healing Catalysis for the Hydrolytic Dehydrogenation of Ammonia Borane

**Fatma Pelin Kinik, Kyriakos Stylianou**

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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,  $\text{NH}_3\text{BH}_3$ ). SION-X is the synthetic form of a mineral and, following in situ reduction, catalyzes the release of almost all 3 equivalents of hydrogen ( $\text{H}_2$ ) 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  $\text{H}_2$  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.

**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; TiB<sub>2</sub>/BN multilayer; thermal stability; heating rate.

**Influence of temperature rise rates on the interfacial structure and mechanical stability of TiB<sub>2</sub>/BN superlattice coatings**

**Dejun Li, Lei Dong**

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The multilayered modulation structure and mechanical properties of TiB<sub>2</sub>/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 TiB<sub>2</sub>/BN multilayers were discussed. The nanoscale TiB<sub>2</sub>/BN multilayers were annealed in vacuum at 700°C for 10, 30, 60 and 120 min. The thermal stability and oxidation resistance of TiB<sub>2</sub>/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 TiB<sub>2</sub>/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.

Thursday, 22/Aug/2019 1:54pm - 2:06pm

**Abstract ID: 690**

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**

**Yeliang WANG**<sup>1,2</sup>

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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 mentioned 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 VSe<sub>2</sub> monolayer[5], semiconducting PtSe<sub>2</sub> monolayer and its intrinsically patterns [6,9], and superconductor transition-metal-trichalcogenide (HfTe<sub>3</sub>)[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 HfTe<sub>3</sub>/HfTe<sub>5</sub> 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.

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

**Abstract ID: 720**

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**

**Wieslaw J Roth**

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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.<sup>1,2</sup> 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.<sup>3</sup> 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 carriers for controlled release studies. Liquid exfoliation<sup>4</sup> 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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Thursday, 22/Aug/2019 8:24am - 8:36am

**Abstract ID: 722**

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  $10\pm 1$  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 10:12am - 10:24am**

**Abstract ID: 723**

**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**

**Huijun Yao**

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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: 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  $\text{Gd}^{3+}$  Incorporation**

**Leelakrishna Reddy, Thabang Nkosi, Balakrishna Avula**

University of Johannesburg, South Africa; [krishr@uj.ac.za](mailto:krishr@uj.ac.za)

$\text{Ca}_3(\text{PO}_4)_2:1\text{Ce}^{3+}/x\text{Gd}^{3+}$  (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  $R3c$ , and several diffraction peaks shifted to lower angle side when co-doped with  $\text{Gd}^{3+}$  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  $\text{Ce}^{3+}$  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  $\text{Gd}^{3+}$  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  $\text{Ce}^{3+}$  ion. The PL spectra showed the intense  $5d-4f$  transition of the  $\text{Ce}^{3+}$  ions with a band maximum at 542 nm, and this band maximum shifted to the longer wavelength region by increasing concentration of the  $\text{Gd}^{3+}$  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  $\text{Gd}^{3+}$  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: 772**

**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**

**Hyuk Jae Jang, Min Seok Kim, Gil Ju Lee, Young Min Song**

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Unlikely 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 SiO<sub>2</sub> mask. First, we grow SiO<sub>2</sub> 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 SiO<sub>2</sub> by reactive ion etching, and Ag removal via HNO<sub>3</sub> solution. Finally, we implement GaN nanostructures by inductively coupled plasma reactive ion etching with SiO<sub>2</sub> mask and buffered oxide etchant for SiO<sub>2</sub> 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**

This work was supported by an Institute for Information & Communications Technology Promotion (IITP) grant funded by the Korea government (MSIP) (No.2017000709)

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Thursday, 22/Aug/2019 8:12am - 8:24am

**Abstract ID: 791**

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**

**Wenbo Xin, Igor M De Rosa, Larry Carlson, Jenn-Ming Yang**

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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.<sup>1-3</sup> 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  $\text{Au}^{3+}$  to  $\text{Au}^0$ , the pre-step for the nucleation of gold clusters.<sup>4</sup> 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.

**Abstract ID: 840**

**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**

**Kausiksankar Das<sup>1</sup>, Benjamin Barnes<sup>2</sup>, Nathan Bane<sup>1</sup>, Ibrahim Elkholy<sup>1</sup>, Samuel Olofin<sup>1</sup>**

<sup>1</sup>University of Maryland Eastern Shore, United States of America; <sup>2</sup>Department of Chemistry and Biochemistry, University of Maryland College Park, United States of America;

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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

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Thursday, 22/Aug/2019 10:52am - 11:04am

**Abstract ID: 846**

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

**Saeed Sameer Ibrahim AlMishal<sup>1</sup>, Tarek Moustafa Hatem<sup>2</sup>, Iman Salah Eldin El-Mahallawi<sup>3</sup>**

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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 CaTiO<sub>3</sub> and BaTiO<sub>3</sub> 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: 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**

**Ying Wang, Sansheng Wang**

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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 HSO<sub>4</sub><sup>-</sup> and SO<sub>4</sub><sup>2-</sup>. 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 m<sup>2</sup>/g and high electrical conductivity of 19.98 S/cm.

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

**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 Ti<sub>2</sub>NiCu Shape Memory Ribbons**

**Pranav Bhale<sup>1</sup>, Pnina Ari-Gur<sup>1</sup>, Victor Koledov<sup>2</sup>, Vladimir Shavrov<sup>2</sup>**

<sup>1</sup>Western Michigan University, United States of America; <sup>2</sup>Kotelnikov Institute of Radio-engineering and Electronics of RAS, 125009 Moscow, Russia; [pnina.ari-gur@wmich.edu](mailto:pnina.ari-gur@wmich.edu)

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 Ti<sub>2</sub>NiCu 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 radiation<sup>1</sup>. The shape-memory performance of the Ti<sub>2</sub>NiCu 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.

#### References

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**Abstract ID: 867**

**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**

**Shuji Nakamura**

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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 Soraa 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 10:20am - 10:50am**

**Abstract ID: 869**

**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**

**Pulickel M. Ajayan**

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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.

**Tuesday, 20/Aug/2019 9:00am - 9:30am**

**Abstract ID: 870**

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

**Keynote**

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

*Keywords:* Transfer technique, Electrohydrodynamic Instability

### **Rapid Large-area Replication of Nanostructures via Pulsed High-voltage Electrohydrodynamic Instability**

**Dae Joon Kang**

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As the conventional lithography confronted the physical barrier in reducing the feature size, intensive efforts for alternative lithographic methods have been dedicated to improving the feasibility of the well-ordered nanostructure fabrication over a large area. Among various types of nanopatterning techniques, electrohydrodynamic lithography (EHL) has been considered a promising tool for replicating nano-sized features in a cost-effective manner. However, EHL is still facing technical challenges to achieve highly faithful pattern replications over a large area. In addition, poor reproducibility, limited pattern height, precise control of parameters, and limited available substrates are the outstanding issues to be resolved. In this regard, we introduced a new lithographic approach based on electrohydrodynamic instability induced by employing pulsed high-voltage ( $> 6.0$  kV) with micro-level air gap ( $> 1.0\mu\text{m}$ ). Compared to the conventional EHL, the high-voltage method (HV-EHL) using stronger electric field ( $> 108\text{V/m}$ ) enhances the overall fidelity including the pattern height. Nonetheless, HV-EHL offsets this influence due to the reduced characteristic time that determines the patterning time for fully-developed pattern. Accordingly, under the non-constant air gap condition, the patterned area can be extended over the entire surface of the resist. To support this, we have confirmed that the parameter constraints for perfect replication is more relieved in HV-EHL, which implies the more facile replication process in our approach. Our pulsed high-voltage EHL is not only a technical improvement but also an innovative lithographic approach to achieve both lithographic requirements and industrial needs by the capability of fabricating a number of functional nanoscale patterns on a large scale in a facile and cost-effective fashion

**Abstract ID: 889**

**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:* Metal Carbides and Nitrides (MXenes)

### **Electronic Properties of 2D Transition Metal Carbides and Nitrides (MXenes)**

**Kanit Hantanasirisakul, Yury Gogotsi**

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2D transition metal carbides and nitrides (MXenes) are a large family of 2D materials with more than 30 compositions experimentally synthesized and a few dozens more predicted to be stable and studied computationally. They benefit from their high electrical conductivity, wide range of optical properties, hydrophilic surface, and high mechanical strength. Because of those properties, they show promise in a wide a variety of applications from energy storage to photonics. In this talk, an overview of fundamental electronic properties of MXenes are presented and discussed. Specifically, the roles of intra- and inter-flake electronic conduction on the temperature-dependence of resistivity of MXenes will be discussed in detail. Moreover, systematic investigation of the roles of MXene composition, including the transition metals, the X elements (C and/or N), and surface terminations on their electronic and transport properties will be presented.

Wednesday, 21/Aug/2019 8:40am - 9:10am

**Abstract ID: 890**

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

**Keynote**

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

*Keywords:* Materials Genome

### **Megalibraries: Expanding and Exploring the Materials Genome**

**Chad A Mirkin**

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Throughout history, the materials we have used and rely on have evolved over time, slowly becoming more and more complex. The progression from the stone tools used by early-man to the polyelemental materials used today has been relatively slow due to the massive parameter space that materials encompass. Indeed, when one considers the 91 metal elements in the periodic table, and all possible combinations, a nearly infinite number of possible materials exist. This is particularly true at the nanoscale where small changes in size or shape, even at a fixed composition, can dramatically change a material's properties. Therefore, the ability to rapidly synthesize and subsequently screen materials for desired properties is needed. In this presentation, a cantilever-free scanning probe lithography approach to combinatorial nanoscience relying on "megalibraries" consisting of as many as 5 billion positionally encoded nanoparticles will be described. The libraries can be tailored to encompass a wide variety of alloy and phase-separated nanoparticles that are comprised of as many as 8 different elements. Importantly, one megalibrary contains more new inorganic materials than scientists cumulatively have produced and characterized to date and can be used to identify new materials and catalysts for important chemical transformations. Additionally, from these libraries, important insight into how thermodynamic phases form in polyelemental nanoparticles has been obtained, and design rules for engineering heterostructures in a polyelemental nanoparticle have been established. Therefore, this novel approach lays the foundation for creating an inflection point in the pace at which we both explore the breadth and discover the capabilities of the materials genome.

**Wednesday, 21/Aug/2019 10:15am - 10:45am**

**Abstract ID: 892**

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

**Keynote**

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

*Keywords:* Meta-Materials

### **Materials by Design: Three-Dimensional (3D) Nano-Architected Meta-Materials**

**J.R. Greer**

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Creation of extremely strong and simultaneously ultra lightweight materials can be achieved by incorporating architecture into material design. In our research, we design and fabricate three-dimensional (3D) nano-architected materials that can exhibit superior and often tunable thermal, photonic, electrochemical, and mechanical properties at extremely low mass densities (lighter than aerogels), which renders them useful, and often enabling, in many scientific pursuits and technological applications. Dominant properties of such meta-materials are driven by their multi-scale nature: from characteristic material microstructure (atoms) to individual constituents (nanometers) to structural components (microns) to overall architectures (millimeters and above). To harness the beneficial properties of 3D nano-architected meta-materials, it is critical to assess their properties at each relevant scale while capturing overall structural complexity. Our research is focused on fabrication and synthesis of such architected materials using 3D lithography, nanofabrication, and additive manufacturing (AM) techniques, as well as on investigating their mechanical, biochemical, electrochemical, electromechanical, and thermal properties as a function of architecture, constituent materials, and microstructural detail. We strive to uncover the synergy between the internal atomic-level microstructure and the nano-sized external dimensionality, where competing material- and structure-induced size effects drive overall response and govern these properties. Specific discussion topics also include their applications in chemical and biological devices, ultra lightweight energy storage systems, damagetolerant fabrics, and smart, multi-functional materials.

Wednesday, 21/Aug/2019 10:45am - 11:15am

**Abstract ID: 893**

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

**Keynote**

*Topics:* Magnetic Materials

*Keywords:* 2D Magnets

## 2D Magnets

**Xiaodong Xu**

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Since the discovery of graphene, the family of two-dimensional (2D) materials has grown to encompass a broad range of electronic properties. However, until recently 2D crystals with intrinsic magnetism were still lacking. Such crystals would enable new ways to study 2D magnetism by harnessing the unique features of atomically-thin materials, such as electrical control for magnetoelectronics and van der Waals (vdW) engineering for novel interface phenomena. In this talk, I will describe our recent magneto-optical spectroscopy experiments on vdW magnets, chromium(III) iodide CrI<sub>3</sub>. I will discuss the layered antiferromagnetic properties of atomically-thin CrI<sub>3</sub> [1,2], electrical control of 2D magnetism [3], giant tunneling magnetoresistance through spin filtering effect in vdW magnetic tunnel junctions [4], and the emerging spin phenomena in vdW magnetic heterostructures [5].

Reference

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## **SYMPOSIUM 6: Functional Thin Films (FTF)**

Thursday, 22/Aug/2019 11:52am - 12:04pm

**Abstract ID: 127**

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, $\text{Ge}_2\text{Sb}_2\text{Te}_5$ (GST)**

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

Otto-von-Guericke-Universität Magdeburg, Germany; [frank.edelmann@ovgu.de](mailto:frank.edelmann@ovgu.de)

This lecture intends to provide an overview of the precursor chemistry that has been developed around the phase-change material germanium-antimony-telluride,  $\text{Ge}_2\text{Sb}_2\text{Te}_5$  (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  $n\text{BuTeTe}n\text{Bu}$  (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).

Thursday, 22/Aug/2019 11:16am - 11:28am

**Abstract ID: 214**

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

**Jingxia Wang**<sup>1,2</sup>

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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(NO<sub>3</sub>)-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 nonwetable wettability[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.

Thursday, 22/Aug/2019 12:04pm - 12:16pm

**Abstract ID: 334**

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**

**Eero Kontturi<sup>1</sup>, Zhuojun Meng<sup>1</sup>, Minna Hakalahti<sup>2</sup>, Elina Niinivaara<sup>1,3</sup>, Tekla Tammelin<sup>1</sup>**

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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.<sup>1</sup> 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 published<sup>2-4</sup> 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 11:40am - 11:52am

**Abstract ID: 339**

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

**Tomasz Runka<sup>1</sup>, Jaroslaw Kaluzny<sup>2</sup>, Wioletta Dewo<sup>1</sup>, Yuriy Zorenko<sup>3</sup>, Vitaliy Gorbenko<sup>3</sup>**

<sup>1</sup>Faculty of Technical Physics, Poznan University of Technology, Poznan, Poland; <sup>2</sup>Faculty of Transport Engineering, Poznan University of Technology, Poznan, Poland; <sup>3</sup>Institute of Physics, Kazimierz Wielki University in Bydgoszcz, Bydgoszcz, Poland;

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Scintillators are special group of materials able to convert high-energy X-rays or  $\gamma$ -rays into photons in UV-visible range. Historically, CaWO<sub>4</sub> 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 CdWO<sub>4</sub> and Bi<sub>4</sub>Ge<sub>3</sub>O<sub>12</sub> scintillators for versatile applications in the field of high-energy physics were popularized [1].

Ce<sup>3+</sup> doped single crystals (SC) of perovskites e.g. YAlO<sub>3</sub> (YAP) and LuAlO<sub>3</sub> (LuAP) have become prevalent for use as scintillators since the 1980's. During the last decade single crystalline films (SCFs) of Ce<sup>3+</sup> doped YAlO<sub>3</sub> [2] and LuAlO<sub>3</sub> [3], as well as the Ce<sup>3+</sup> and Mn<sup>2+</sup> doped TbAlO<sub>3</sub> (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, Mn<sup>2+</sup> doped TbAP and Ce<sup>3+</sup> 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 Y<sup>3+</sup> ions by Tb<sup>3+</sup> or Lu<sup>3+</sup> 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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Thursday, 22/Aug/2019 11:04am - 11:16am

**Abstract ID: 359**

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Sol-gel and LB technology

Keywords: SiO<sub>2</sub>, thin films, barrier coatings, high pressure vessels

### **Organically Functionalized Sol-Gel Silica Coatings on Polymers For Reduction Of Gas Leakage**

**Anna Szczurek, Jerzy Kaleta, Justyna Krzak**

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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.

**Wednesday, 21/Aug/2019 1:36pm - 1:48pm**

**Abstract ID: 360**

**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**

**Jasper Joost Michels**

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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.

Thursday, 22/Aug/2019 12:28pm - 12:40pm

**Abstract ID: 370**

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**

**Khadijah Thibodeaux<sup>1,2</sup>, Gabriella Kimmerly<sup>1,3</sup>, Bethany Reim<sup>1,4</sup>, Jensina Froland<sup>1,3</sup>,  
Babak Sani<sup>1,3,4,5</sup>**

<sup>1</sup>Keck Science Department, Claremont, CA; <sup>2</sup>Pomona College, Claremont, CA, USA; <sup>3</sup>Scripps College, Claremont, CA, USA; <sup>4</sup>Pitzer College, Claremont, CA, USA; <sup>5</sup>Claremont McKenna College, Claremont, CA, USA; [bsanii@kecksci.claremont.edu](mailto:bsanii@kecksci.claremont.edu)

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 12:40pm - 12:52pm

**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**

**Tekla Tammelin<sup>1</sup>, Matti Putkonen<sup>1</sup>, Marie Gestranus<sup>1</sup>, Maarit Karppinen<sup>2</sup>, Eero Kontturi<sup>2</sup>**

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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.<sup>1</sup> 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.<sup>2</sup> Inorganic multilayer structures comprising stacks of SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> deposited on CNF film (individual layer thickness of 3.7 nm for SiO<sub>2</sub> and 2.6 nm for and Al<sub>2</sub>O<sub>3</sub>) efficiently blocked the diffusion of the oxygen molecules through the CNF film structure.<sup>3</sup> Moreover, simultaneously developed low temperature ALD processes enabled the inorganic thin film depositions on thermally sensitive biomaterials.

Wednesday, 21/Aug/2019 2:48pm - 3:00pm

**Abstract ID: 402**

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**

**Haiping Gao, Xin Tong, Su Liu, Bopeng Zhang, Yongsheng Chen**

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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/m<sup>2</sup> 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.

Wednesday, 21/Aug/2019 1:12pm - 1:24pm

**Abstract ID: 404**

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**

**Shengjie Zhai, Yihong Zhao, Hui Zhao**

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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 programing the quasi-random sequence consisting of 0s and 1s, we can create the quasi-random nanostructures on the optical disc from Fibonacci and Rudio-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 Rudio-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 photonvatics, our programmable quasi-random nanostructures with exceptional broadband and omnidirectional photon management can find important applications in broad-band LEDs and optoelectronic devices.

Wednesday, 21/Aug/2019 2:12pm - 2:24pm

**Abstract ID: 418**

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Ferroelectric film

Keywords: Ferroelectricity, HfO<sub>2</sub>, Thin film, Phase transformation, Memory

### **Appearance and Disappearance of Ferroelectric Phase in Crystalline HfO<sub>2</sub> Thin Films Induced by Annealing Procedure**

**Shinji Migita, Hiroyuki Ota**

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Amorphous phase HfO<sub>2</sub> thin films are nowadays utilized as the high-k gate dielectric film of advanced field-effect transistors in large-scale integrated circuits (LSI). Once HfO<sub>2</sub> films are crystalized, they present interesting dielectric properties depending on their crystal phases. HfO<sub>2</sub> crystals are metamorphic and have cubic, tetragonal, orthorhombic, and monoclinic structures. Among the multiphase of HfO<sub>2</sub> crystals the orthorhombic crystal phase show ferroelectricity [1]. The effective ways for the formation of orthorhombic phase are doping metals into HfO<sub>2</sub> 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 HfO<sub>2</sub> 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 HfO<sub>2</sub> thin films.

Thursday, 22/Aug/2019 10:52am - 11:04am

**Abstract ID: 447**

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**

**Yong Tae PARK<sup>1</sup>, Dongseob KIM<sup>2</sup>, Kyungwho CHOI<sup>3</sup>, Dukhyun CHOI<sup>4</sup>**

<sup>1</sup>Myongji University, Korea, Republic of (South Korea); <sup>2</sup>KITECH, Korea, Republic of (South Korea); <sup>3</sup>Korea Railroad Research Institute, Korea, Republic of (South Korea); <sup>4</sup>Kyung Hee University, Korea, Republic of (South Korea); [ypark@mju.ac.kr](mailto:ypark@mju.ac.kr)

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.

Thursday, 22/Aug/2019 3:30pm - 3:42pm

**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**

**Simonas Ramanavicius, Arunas Jagminas**

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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.

Thursday, 22/Aug/2019 1:04pm - 1:16pm

**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**

**Yaron Paz, Omry Dinner, Gideon Grader**

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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.

Thursday, 22/Aug/2019 12:16pm - 12:28pm

**Abstract ID: 476**

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**

**Stefan Seeger, Sandro Oliveira, Georg Artus, Naeem Saddiqi**

University of Zurich, Switzerland; [sseeger@chem.uzh.ch](mailto:sseeger@chem.uzh.ch)

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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Wednesday, 21/Aug/2019 2:00pm - 2:12pm

**Abstract ID: 534**

Symposium 6: Functional Thin Films (FTF)

Poster 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**

**Jozef Huran<sup>1,5</sup>, Pavol Bohacek<sup>1</sup>, Vlasta Sasinkova<sup>2</sup>, Angela Kleinova<sup>3</sup>, Miroslav Mikolasek<sup>4</sup>, Alexander P. Kobzev<sup>5</sup>, Maria Sekacova<sup>1</sup>, Juraj Arbet<sup>1</sup>**

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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 SiH<sub>4</sub> (100 %), CH<sub>4</sub> (100 %) and PH<sub>3</sub> (2 vol. % in H<sub>2</sub>) or B<sub>2</sub>H<sub>6</sub> (5 vol. % in H<sub>2</sub>) as precursor gasses and H<sub>2</sub> 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.

Thursday, 22/Aug/2019 11:28am - 11:40am

**Abstract ID: 596**

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**

#### **Libor Juha**

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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  $\sim 70$  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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Wednesday, 21/Aug/2019 1:24pm - 1:36pm

**Abstract ID: 599**

Symposium 6: Functional Thin Films (FTF)

Oral Presentation

Topics: Metal oxide, carbon, nitrides etc based thins Films

Keywords: TiO<sub>2</sub>, CuO, Heterostructures, Thin Films, Gas Sensing

### CuO/TiO<sub>2</sub> p-n Thin Film Nanoheterostructures for Gas Sensing Applications

**Katarzyna Ewa Zakrzewska<sup>1</sup>, Wojciech Maziarz<sup>1</sup>, Marta Radecka<sup>2</sup>, Michał Mazur<sup>3</sup>,  
Damian Wojcieszak<sup>3</sup>, Danuta Kaczmarek<sup>3</sup>**

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CuO/TiO<sub>2</sub> 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 H<sub>2</sub> at 300°C for the multiple-networked TiO<sub>2</sub>-decorated CuO nanorod films. In our contribution, we demonstrate CuO and CuO/TiO<sub>2</sub> 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 TiO<sub>2</sub> layers (Fig.2). Bi-layered heterostructures synthesized on special gas sensor substrates with precisely defined interdigital electrodes were tested towards NO<sub>2</sub> 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 TiO<sub>2</sub> 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/TiO<sub>2</sub> Fig.2 Elemental mapping of CuO/TiO<sub>2</sub> thin thin film film

Key Words: TiO<sub>2</sub>, CuO, Heterostructures, Thin Films, Gas Sensing

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Wednesday, 21/Aug/2019 2:36pm - 2:48pm

**Abstract ID: 609**

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 $\pi$ -Delocalized Radicals

**Kilingaru I. Shivakumar<sup>1</sup>, Szymon Kapusciński<sup>2</sup>, Marcin Jasiński<sup>2</sup>, Martin Cigl<sup>1</sup>, Jacek Szczytko<sup>3</sup>, Hirosato Monobe<sup>4</sup>, Damian Pocięcha<sup>5</sup>, Piotr Kaszyński<sup>1,2,6</sup>**

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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  $\pi$ -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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Wednesday, 21/Aug/2019 3:24pm - 3:36pm

**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 Ta<sub>2</sub>O<sub>5</sub> Films Synthesized By Co-Sputtering And De-Alloying Approach**

**Jang-Hsing Hsieh<sup>1</sup>, S. H. Wu<sup>1</sup>, C. Li<sup>2</sup>, Y. C. Lin<sup>1</sup>**

<sup>1</sup>Ming Chi University of Technology, Taiwan; <sup>2</sup>National Yang Ming University;

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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.

Wednesday, 21/Aug/2019 2:24pm - 2:36pm

**Abstract ID: 641**

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**

**Zhijia Yu**

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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. Heat transfer and fluid flow of water flowing laminarly 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.

Thursday, 22/Aug/2019 10:40am - 10:52am

**Abstract ID: 672**

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**

**Muhammad Hanis Tajuddin<sup>1,2</sup>, Norhaniza Yusof<sup>1,2</sup>, Wan Norharyati Wan Salleh<sup>1,2</sup>, Ahmad Fauzi Ismail<sup>1,2</sup>, Juhana Jaafar<sup>1,2</sup>, Farhana Aziz<sup>1,2</sup>**

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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 (Na<sub>2</sub>SO<sub>4</sub>) by cross flow filtration system. The best performance NF membrane was (TFN 0.05) with high water flux and MgCl<sub>2</sub> rejection with values of 27.18 L/m<sup>2</sup>.h and 95.98% respectively. This study has experimentally validated the potential of LDH materials in membrane process for improvement in water separation process.

**Wednesday, 21/Aug/2019 1:00pm - 1:12pm**

**Abstract ID: 707**

**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**

**Ke-Qing Zhao**

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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.

Wednesday, 21/Aug/2019 1:48pm - 2:00pm

**Abstract ID: 713**

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: 797**

**Symposium 6: Functional Thin Films (FTF)**

**Poster Presentation**

*Topics:* Thin Film Growth & Epitaxy

*Keywords:*  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub>; MOCVD; heteroepitaxy; phase transition.

### **Heteroepitaxy of $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub> thin films by metal organic chemical vapor deposition**

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The research interest in Ga<sub>2</sub>O<sub>3</sub> materials is inspired by its ultra-wide bandgap of ~4.9 eV. Baliga's figure of merit for Ga<sub>2</sub>O<sub>3</sub> is several times higher than that of GaN and SiC, allowing Ga<sub>2</sub>O<sub>3</sub> 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  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub> due to polarization effect, which contributes to the realization of high mobility  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub>-based devices [2]. However, 1) the growth of  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub> thin films are always mixed by  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> and 2) the crystal quality of  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub> grown by heterogeneous substrates are low [3, 4]. In this work, Ga<sub>2</sub>O<sub>3</sub> thin films were grown by metal organic chemical vapor deposition (MOCVD) using O<sub>2</sub>, H<sub>2</sub>O, N<sub>2</sub>O as oxygen precursors. The temperature range was set to 450~660 °C and the phase transition and phase stability of  $\beta$ - and  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub> were investigated. It is found that phase pure  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub> easily forms on c-plane sapphire substrates by using Triethylgallium (TEGa) and H<sub>2</sub>O 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  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub> was effectively improved. The growth mode of  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub> changed from 3D multi-layer mode to 2D layer-by-layer mode as the temperature raised. We derive high quality  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub> 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  $1.8 \times 10^8$  cm<sup>-2</sup>. Nowadays, large-size sapphire is commercially available and cheap. Using sapphire as the substrate for  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub> could lower the cost of  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub>-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  $\epsilon$ -Ga<sub>2</sub>O<sub>3</sub>-based materials and devices.

**Abstract ID: 817**

**Symposium 6: Functional Thin Films (FTF)**

**Poster Presentation**

*Topics:* Thin Film Growth & Epitaxy

*Keywords:* composite films, Ar/O<sub>2</sub> ratio, CaZrO<sub>3</sub>, surface morphology, crystal structure, RF sputtering

**The effects of Ar/O<sub>2</sub> ratio on the structure and properties of CaZrO<sub>3</sub>/Ca<sub>0.15</sub>Zr<sub>0.85</sub>O<sub>1.85</sub> composite films**

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The CaZrO<sub>3</sub>/Ca<sub>0.15</sub>Zr<sub>0.85</sub>O<sub>1.85</sub> composite films have been prepared using the by the radio-frequency (RF) magnetron sputtering under the different ratios of Ar/O<sub>2</sub>. We have studied the effects of the different gas concentrations (Ar/O<sub>2</sub>) on a crystal structure, a surface morphology, and electrical properties of the CaZrO<sub>3</sub>/Ca<sub>0.15</sub>Zr<sub>0.85</sub>O<sub>1.85</sub> 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/O<sub>2</sub> ratio results in an improvement of the structural quality of the CaZrO<sub>3</sub> films and the reduction of Ca<sub>0.15</sub>Zr<sub>0.85</sub>O<sub>1.85</sub> phase. Further, increasing Ar/O<sub>2</sub> ratio results in an increase in surface roughness and grain size for the as-deposited samples.

Thursday, 22/Aug/2019 12:52pm - 1:04pm

**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 VO<sub>2</sub> 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 VO<sub>2</sub>-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 VO<sub>2</sub>-based actuators using the thermal properties of VO<sub>2</sub>, 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: 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  
REBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$</sub>  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 REBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$</sub>  (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 REBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$</sub>  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 REBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$</sub>  thin films.

Wednesday, 21/Aug/2019 3:00pm - 3:12pm

**Abstract ID: 871**

Symposium 6: Functional Thin Films (FTF)

**Invited Talk**

*Topics:* Thin films for optoelectronics, nanoelectronics and spintronics

*Keywords:* diamond ; nitrogen vacancy ; color centers; oxygen regulation; emission

**Efficient regulation of nitrogen-vacancy center ensembles in diamond through nitrogen-oxygen co-doping technique**

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Quantum emitters in solid-state systems such as nitrogen-vacancy (NV) color centers embedded in diamond are crucial to the development of quantum information processing, integrated photonics and advanced sensing. However, a remaining challenge is how to regulate NV centers with uniform spatial distribution and higher density. Here, we demonstrate that the distribution and intensity of NV centers can be efficiently tailored by using an in situ nitrogen-oxygen co-doping technique with fixed nitrogen concentrations during MPCVD. By the engineering of oxygen flow into the H<sub>2</sub>/CH<sub>4</sub>/N<sub>2</sub> plasma, we find that lower oxygen concentrations contribute to the formation of NV centers, while higher oxygen concentrations will hinder the formation of NV centers. There is a great correlation between the regulating effects of oxygen on NV centers and the quality improvement of diamond films. The intensity of diamond NV centers is the net result of the competition mechanism between the increasing PL intensity caused by the formation of NV color centers and the quenching PL intensity due to the non-radiative recombination of photo-excited NV color centers induced by the degradation of crystalline quality of the as-grown diamond films with higher oxygen contents. Furthermore, first-principles calculations provide evidence that oxygen impurities tend to exist in the diamond NV systems in the form of interstitial atoms, and the formation energies of different oxygen concentrations undergo a process of decreasing first and then increasing. The calculation results are in good agreement with the experimental observations, indicating the accurate rule of oxygen regulation. The proposed method may provide an alternative platform for designing a range of stable, room temperature single photon source with controllably intensity and spatial distribution.

Wednesday, 21/Aug/2019 3:12pm - 3:24pm

**Abstract ID: 873**

Symposium 6: Functional Thin Films (FTF)

**Oral Presentation**

*Topics:* Thin Film Growth & Epitaxy

*Keywords:* Ag<sub>2</sub>Se, topological insulators, topological surface states, molecular beam epitaxy, scanning tunneling microscopy

### Scanning Tunneling Microscopy Study of the Possible Topological Surface States in MBE Grown Ag<sub>2</sub>Se

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Scanning tunneling microscopy study of the possible topological surface states in MBE grown Ag<sub>2</sub>Se

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Topological surface states (TSSs) are a class of novel electronic states that are of potential interest in quantum computing or spintronic applications. Unlike conventional two-dimensional electron states, these surface states are expected to be immune to localization and to overcome barriers caused by material imperfection<sup>1</sup>. The formation of spin-textured metallic edge states in Topological Insulators (TIs) enables highly coherent charge and spin transport, making them promising for spintronic applications<sup>2</sup>. TSSs with highly anisotropic Dirac cones, are theoretically expected in silver chalcogenides (Ag<sub>2</sub>Se and Ag<sub>2</sub>Te)<sup>2</sup>.

Epitaxial layers of  $\beta$ -Ag<sub>2</sub>Se nanostructures, a new class of 3D TIs, were synthesized using molecular beam epitaxy (MBE) method using elemental Ag and Se sources. The growth was combined with in situ high energy electron diffraction (RHEED). High-temperature single stage growth regime was adopted to fabricate Ag<sub>2</sub>Se layers. As confirmed by the scanning tunneling microscopy (STM), the surface of Ag<sub>2</sub>Se layers consists of closely spaced nanometer sized islands with dimensions dependent on the growth time on which thin films grow well in an island growth mode. Based on atomic-resolution STM images, a new monoclinic structure is proposed for the MBE grown Ag<sub>2</sub>Se film, which was not seen in this system before. As shown by STM analysis, the Ag<sub>2</sub>Se layers possess two different monoclinic and orthorhombic crystal structures with the majority of monoclinic structure. It was further shown that (111) plane of the orthorhombic structure always coexists with the (001) plane of the monoclinic structure providing a bold atomic pattern due to their height difference. The electronic structure of both coexisted atomic structures of the Ag<sub>2</sub>Se have been investigated by means of scanning tunneling spectroscopy (STS). To test the unique feature of TSSs, we have used STM to examine Ag<sub>2</sub>Se surface states and to measure their reflection by and transmission through atomic steps. This study can provide valuable insight

into their exotic electrical properties and may allow their possible applications for spintronics and quantum information applications.

Key words: Ag<sub>2</sub>Se, topological insulators, topological surface states, molecular beam epitaxy, scanning tunneling microscopy

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**Abstract ID: 882**

**Symposium 6: Functional Thin Films (FTF)**

**Oral Presentation**

*Topics:* Organic and polymer film

*Keywords:* Pressure Sensor, Conducting Polymer, Micro-pyramid

**A Highly Sensitive and Stable Pressure Sensor by Conformal Nano-coating on  
Micro-pyramid arrays using Conducting Polymer**

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Sunjong Lee<sup>2</sup>, Sunkook Kim<sup>1</sup>**

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Conducting polymer is widely used in many fields such as electric device, energy conversion device, supercapacitor, various sensors and energy storage system because of its high electric conductivity, easy process and availability, and easy mass synthesis characteristics and has been undergoing research and development. 1-3 Electrical resistive pressure sensors are fabricated by coating conductors on uneven surfaces such as arrays of pyramids or domes. In order to obtain a stable resistive change by repetitive pressure, the conductor must have non-rigid flexibility. In this regard, flexible conductive polymers are the best materials for their conductors. Therefore, in this study, the conductive polymer was used as a conductor used as a sensing material of a pressure sensor. The electrical characteristics of pressure sensitivity, stability, and responsiveness of the fabricated pressure sensor were analyzed. Also, it has been applied to blood pressure sensor and its superior detection power shows that this pressure sensor has excellent characteristics for a commercialization.