

## 3<sup>rd</sup> International Conference on Material Science & Nanotechnology

### Keynote Talks

#### Smart Soft Materials in Tissue Engineering and Soft Robotics

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#### Abstract

The synthesis of different hydrophilic polymeric networks, by in situ radical polymerization in the presence of graphene derivatives, gives rise to three-dimensional nanocomposite soft structures. The role of the nanomaterial within the polymer network is primarily intended for the reinforcing (i.e., increasing the stiffness and toughness). However, we have shown that the presence of graphene can also enhance features such as biocompatibility and sensing, giving rise to truly hybrid composites. In this talk we will discuss the development of these polymeric networks as smart soft materials that emulate the mechanical properties of living tissues, as well as their ability to self-heal. In addition, their response to different stimuli, such as electric and magnetic fields, and the possibility of preparation following 3D printing methodologies, paves the way for applications in two large and currently highly relevant fields: tissue engineering and drug delivery.

#### 2D Nanostructures at Atomic Scale: from Energy and Environmental Applications to Quantum Devices

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#### Abstract

Technology at the nanoscale has become one of the main challenges in science as new physical effects appear and can be modulated at will. As developments in materials science are pushing to the size limits of physics and chemistry, there is a critical need for understanding the origin of these unique properties and relate them to the changes originated at the atomic scale, e.g.: linked to structural changes of the material, many times related to the presence of crystal defects or crystal surface terminations. Especially on 2D materials designed for electrocatalysis in energy and environmental applications, crystallography and distribution of the atomic species are of utmost importance in order to determine the active sites that will improve the reaction performance, including efficiency and selectivity towards certain reactions. In 2D nanomaterials the distribution and coordination of metal species at the surface are determining their final electrocatalytic behavior as the reactions of interest mainly occur at the surface. The presentation will show how pristine and perfect crystalline surfaces may tend to be inert versus certain reactions, while creation of certain types of defects or even a predetermined surface amorphization may highly improve the catalytic activity of these 2D nanomaterials.

In the present work, I will show how combining advanced electron microscopy imaging with electron spectroscopy, in an aberration corrected STEM will allow us to probe the elemental composition and structure in unprecedented spatial detail, while determining the growth mechanisms and correlating the structural properties to their electrocatalytic performance.

## Graphene Coatings: A Disruptive Approach to Remarkable Corrosion Resistance

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### Abstract

Corrosion and its mitigation costs dearly (any developed economy loses 3-4% of GDP due to corrosion, which translates to ~\$250b to annual loss USA). In spite of traditional approaches of corrosion mitigation (e.g., use of corrosion resistance alloys such as stainless steels and coatings), loss of infrastructure due to corrosion continues to be a vexing problem. So, it is technologically as well as commercially attractive to explore disruptive approaches for durable corrosion resistance.

Graphene has triggered unprecedented research excitement for its exceptional characteristics. The most relevant properties of graphene as corrosion resistance barrier are its remarkable chemical inertness, impermeability and toughness, i.e., the requirements of an ideal surface barrier coating for corrosion resistance. However, the extent of corrosion resistance has been found to vary considerably in different studies. The author's group has demonstrated an ultra-thin graphene coating to improve corrosion resistance of copper by two orders of magnitude in an aggressive chloride solution (i.e., similar to sea-water). In contrast, other reports suggest the graphene coating to actually enhance corrosion rate of copper, particularly during extended exposures. Authors group has investigated the reasons for such contrast in corrosion resistance due to graphene coating as reported by different researchers. On the basis of the findings, author's group has succeeded in demonstration of durable corrosion resistance as result of development of suitable graphene coating. The presentation will also assess the challenges in developing corrosion resistant graphene coating on most common engineering alloys, such as mild steel, and presents results demonstrating circumvention of these challenges.

## Flexible Thermoelectrics

Lidong Chen

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### Abstract

Flexible thermoelectrics provides a different solution for developing portable and sustainable flexible power supplies. The discovery of Ag<sub>2</sub>S-based ductile semiconductors has driven a shift in the potential for flexible thermoelectrics, but the lack of good ductile thermoelectric materials has restricted the reality of fabricating conventional cross-plane  $\pi$ -shape flexible devices. We report a series of high-performance n- and p-type ductile thermoelectric materials based on the composition-performance phase diagram in AgCu(Se,S,Te) pseudo-ternary solid solutions, with high- $zT$  values of  $>0.5$  at room temperature. We further demonstrated thin and flexible  $\pi$ -shape devices with a maximum normalized power density of  $>30 \mu\text{Wcm}^{-2}\text{K}^{-2}$ . This output is promising for the usage of flexible thermoelectrics in wearable electronics.

## Heterostructured Material: New Science Produces Superior Properties

Yuntian Zhu

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## Abstract

Strong and tough materials are desired for light-weight applications such as electric cars and aerospace applications. Recently, heterostructures are found to produce unprecedented strength and ductility that are considered impossible from our textbook knowledge and materials history. Heterostructured materials consist of heterogeneous zones with dramatic (>100%) variations in mechanical and/or physical properties. The interaction in these hetero-zones produces a synergistic effect where the integrated property exceeds the prediction by the rule-of-mixtures. Importantly, HS materials can be produced by current industrial facilities at large scale and low cost. There are many scientific issues with such materials that challenge the communities of experimental materials science and computational material mechanics. Heterostructured materials is quickly becoming a hot research field in the post-nanomaterials era. In this talk I'll present the current advances as well as future challenges and issues in this emerging field.

## Design, Preparation and Characterization of Functional Nanomaterials Based on Energy-resolved Distribution of Electron Traps

Bunsho Ohtani

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## Abstract

How can we design functional solid materials, such as catalysts and photocatalysts? What is the decisive structural parameters controlling their activities, performance or properties? What is obtained as structural properties by popular conventional analytical methods, such as X-ray diffraction (XRD) or nitrogen-adsorption measurement, is limited to bulk crystalline structure and specific surface area, i.e., no structural characterization on amorphous phases, if present, and surface structure has been made so far. This is because there have been no macroscopic analytical methods to give surface structural information including possibly-present amorphous phases. Recently, we have developed reversed double-beam photoacoustic spectroscopy (RDBPAS) which enables measure energy-resolved distribution of electron traps (ERDT) for semiconducting materials such as metal oxides. Those detected electron traps (ETs) seem to be predominantly located on the surface for almost all the metal oxide particles, and therefore they reflect macroscopic surface structure, including amorphous phases, in ERDT patterns. Using an ERDT pattern with the data of CB bottom position (CBB), i.e., ERDT/CBB pattern, it has been shown that metal oxide powders, and the other semiconducting materials such as carbon nitride, can be identified without using the other analytical data such as XRD patterns or specific surface area, and similarity/differentness of a pair of metal-oxide samples is quantitatively evaluated as degree of coincidence of ERDT/CBB patterns. An approach of material design based on the ERDT/CBB analyses is introduced.

## Chemically Modified Graphene for Real-world Applications

Sang Ouk Kim

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## Abstract

Graphene Oxide Liquid Crystal (GOLC) is an intriguing 2D carbon based soft material, which exhibits nematic type colloidal discotic liquid crystallinity with the orientational ordering of graphene oxide flakes in good solvents, including water. Since our first discovery of GOLC in aqueous dispersion at 2009, this interesting mesophase has been utilized over world-wide for many different application fields, such as liquid crystalline graphene fiber spinning, highly ordered graphene membrane/film production, prototype liquid crystal display and so on. Interestingly, GOLC also allow us a valuable opportunity for the highly ordered molecular scale assembly of functional nanoscale structures. This presentation will introduce our current status of GOLC research particularly focusing on the nanoscale assembly of functional nanostructures, including highly oriented 1D fibers, 2D films and 3D nanoporous

structures. Besides, relevant research works associated to the nanoscale assembly and chemical modification of various low dimensional materials, including 1D carbon nanotubes, 2D TMDs and MXene, will be presented particularly aiming at energy and environmental applications. In the last part of presentation, our first discovery of single atom catalyst will be introduced also, including other relevant research efforts exploiting the customized heteroelement doping of graphene-based structures.

## **Engineering at the Nanoscale: A Strategy for Developing High Performance Functional Materials**

**Sabu Thomas**

*Mahatma Gandhi University, India*

### **Abstract**

Green chemistry started for the search of benign methods for the development of nanoparticles from nature and their use in the field of antibacterial, antioxidant, and antitumor applications. Bio wastes are eco-friendly starting materials to produce typical nanoparticles with well-defined chemical composition, size, and morphology. Cellulose, starch, chitin and chitosan are the most abundant biopolymers around the world. Cellulose nanoparticles (fibers, crystals and whiskers) can be extracted from agrowaste resources. Chitin is the second most abundant biopolymer after cellulose, it is a characteristic component of the cell walls of fungi, the exoskeletons of arthropods and nanoparticles of chitin (fibers, whiskers) can be extracted from shrimp and crab shells. Starch nano particles can be extracted from tapioca and potato wastes. These nanoparticles can be converted into smart and functional biomaterials by functionalization through chemical modifications due to presence of large amount of hydroxyl group on the surface. The preparation of these nanoparticles includes both series of chemical as well as mechanical treatments, crushing, grinding, alkali, bleaching and acid treatments. Since large quantities of bio wastes are produced annually, further utilization of cellulose, starch and chitins as functionalized materials is very much desired. The cellulose, starch and chitin nano particles are currently obtained as aqueous suspensions which are used as reinforcing additives for high performance environment-friendly biodegradable polymer materials. These nanocomposites are being used as biomedical composites for drug/gene delivery, nano scaffolds in tissue engineering and cosmetic orthodontics. The reinforcing effect of these nanoparticles results from the formation of a percolating network based on hydrogen bonding forces. The incorporation of these nano particles in several bio-based polymers have been discussed. The role of nano particle dispersion, distribution, interfacial adhesion and orientation on the properties of the ecofriendly bio nanocomposites have been carefully evaluated.

## **Session: Nanomaterials**

### **Featured Presentations**

### **3D Visualization Method Based on Metastructure Optical Indicator of Thermoelastic Polarization Microscope for Electromagnetic Fields in Microwave and THz Ranges**

**A. Babajanyan<sup>a\*</sup>, Zh. Baghdasaryan<sup>b</sup>, H. Parsamyan<sup>a</sup>, B. Friedman<sup>c</sup>, and K. Lee<sup>b</sup>**

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<sup>b</sup>*Department of Physics, Sogang University, South Korea*

<sup>c</sup>*Department of Physics, Sam Houston State University, Huntsville, USA*

### **Abstract**

Noncontact visualization technique for the electric and magnetic near-field distributions in microwave and THz ranges were performed using the thermoelastic optical indicator polarization microscopy (TEOIPM). New optical indicators based on periodic dielectric-metal metaelements were designed for separate electric and magnetic fields

visualization. Depending on the orientation and ordering of the structure, such metastructure-based indicators allow separately visualize the x- and y-components of the in-plane electric as well as magnetic fields for anisotropic materials. Numerical simulations were provided to optimize the characterization efficiency of the designed metastructures. In addition, the 3D visualization of the microwave near-field distribution was built, to show the field intensity and shape distribution dependencies on the distance from the electromagnetic source.

## Resonant Interaction Between Microwaves and Thin Conducting Microstructure with Finite Length

T. Abrahamyan<sup>a</sup>, H. Haroyan<sup>a</sup>, D. Hambaryan<sup>a</sup>, H. Parsamyan<sup>a</sup>, K. Lee<sup>b</sup>, A. Babajanyan<sup>a</sup> and Kh. Nerkararyan<sup>a</sup>

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<sup>b</sup>Department of Physics, Sogang University, South Korea

### Abstract

A thermoelastic optical indicator microscope (TEOIM) was used to characterize the thin conducting microstructures with a length of several half-wavelengths which serves as a resonator for axial surface waves. The presence of a weak axial electric field component of surface waves ensures an easy coupling with the incident plane microwaves ((8–12 GHz) polarized along the rod axis and excites the resonator. Visualization of distributions of the near-field magnetic component of surface standing waves in the vicinity of a rod allows one to explore several longitudinal modes of a resonator with low orders. Increasing the conductivity of a rod ensures efficient excitation of the resonator by a linearly polarized plane wave incident perpendicular to a rod axis. Decreasing a rod diameter results in an increase of reflections from the rod edges and as a consequence the wave intensity increases. The Q-factor is of the order of ten for low order modes. Interaction between a graphite-based microstrip as element of a metamaterial, and incident microwaves in X-band was investigated. The distribution of the magnetic near-field visualized by a TEOIM has several localization centers which depend on the conductivity and sizes of the graphite microstrip. The superposition of incident and scattered waves reveals a significant phase-shift in the scattered wave due to a change in the complex conductivity of the graphite. A microstructure consisting of metaelements with such regulated conductivity can serve as a phase-tuning tool for EM wave control.

## Sprayed Nanometer-thick Hard Magnetic Coatings with Strong Perpendicular Anisotropy for Data-storage Applications

A. Chumakov<sup>a\*</sup>, C.J. Brett<sup>a,b</sup>, K. Gordeyeva<sup>b</sup>, D. Menzel<sup>c</sup>, L.O.O. Akinsinde<sup>d,e</sup>, M. Gensch<sup>a</sup>, M. Schwartzkopf<sup>a</sup>, W. Cao<sup>f</sup>, S. Yin<sup>f</sup>, M.A. Reus<sup>f</sup>, M.A. Rübhausen<sup>d</sup>, P. Müller-Buschbaum<sup>f</sup>, L. D. Söderberg<sup>b</sup> and S.V. Roth<sup>a,b</sup>

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### Abstract

We present a study of a facile technology for establishing mono- and multilayer nanostructures made from single-domain flat magnetic nanoparticles (MNPs). MNPs exhibit a strong perpendicular-oriented magnetic moment on solid and flexible substrates. Surfactant-free, ferromagnetic SrFe<sub>12</sub>O<sub>19</sub> nanoparticles with perpendicular magnetic moment orientation and two different aspect ratios are self-ordered into thin nanofilms exploiting the templating effect of cellulose nanofibrils, and magnetic fields. Uniform magnetic coatings obtained by scalable layer-by-layer

spray deposition from a monolayer coverage up to thicknesses of a few tens of nanometers show preferred in-plane orientation of the hard-magnetic nanoparticles. Using grazing incidence X-ray scattering, we quantify the self-assembly during deposition and the MNPs stacking into three-dimensional multilayer structures. Application of the magnetic field during film deposition ensures additional improvement in perpendicular magnetic anisotropy.

## Titania Supported Silver-Nickle Visible Light Photocatalyst for Environmental and Health Applications

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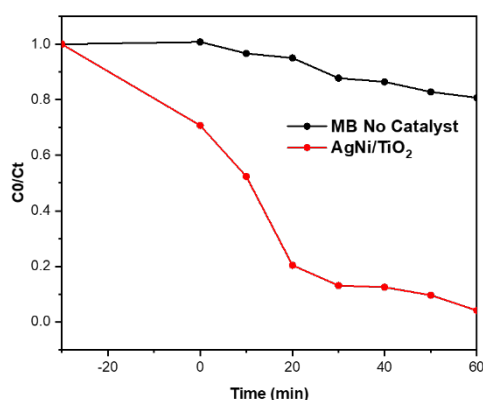
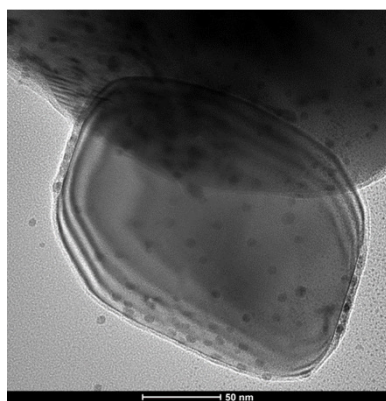
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### Abstract

Water pollution caused by industrial waste and the growth of bacteria and viruses on surfaces of materials has become major problems in recent years. Heterogeneous semiconductor-based photocatalysts such as Ag, Ni, and AgNi supported on TiO<sub>2</sub> or ZnO offer a cost-effective solution due to their superior photocatalytic degradation properties and anti-microbial activity. In this work, we report the synthesis and characterization of AgNi/TiO<sub>2</sub> nanocomposites for visible-light photocatalytic and anti-microbial applications. Our analysis showed that a small silver nanoparticle is well-dispersed on the surface of nickel oxide and Titania. The photocatalytic degradation efficiency toward Methylene Blue (M.B.) dye in the aqueous suspensions of AgNi/TiO<sub>2</sub> under visible light irradiation exhibited superior catalytic activity compared to Ag/TiO<sub>2</sub>, Ni/TiO<sub>2</sub>, and bare TiO<sub>2</sub>. Annealing of AgNi/TiO<sub>2</sub> nanocomposites has shown a faster degradation of M.B., where the degradation efficiency reaches 95.92% in less than 60 minutes of degradation time. Furthermore, synthesized photocatalysts showed high degradation efficiency and significant inhibition of microorganisms such as Gram-negative E. Coli and Gram-positive S. aureus, which makes it an effective photocatalyst for wastewater treatment and disinfectant for surfaces and anti-microbial textiles.



## Fabrication of Au Nanoparticles Supported on One-dimensional (1D) La<sub>2</sub>O<sub>3</sub> Nanorods for Selective Esterification of Methacrolein to Methyl Methacrylate with Molecular Oxygen

Bappi Paul

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## Abstract

Here we demonstrate a simple and cost-effective synthetic route for selective esterification of aldehydes with high productivity in the presence of molecular oxygen ( $O_2$ ) on gold supported lanthanum oxide ( $Au/La_2O_3$ ) nanoparticle catalyst. Au nanoparticles with sizes of 2–7 nm supported on 1D  $La_2O_3$  nanorods with diameters between 20 and 50 nm was synthesized by room-temperature surfactant-assisted single-step preparation method. The as-synthesized catalyst was thoroughly characterized by powder XRD, SEM, HR-TEM, H<sub>2</sub>-TPR, XPS, TGA/DTA, FTIR, BET, EXAFS and UV-visible spectroscopy. This prepared nanostructured catalyst was found to be highly effective in liquid phase production of methyl methacrylate through direct oxidative esterification of methacrolein with high turnover number of ~1136. The effect of various reaction controlling parameters like reaction temperature, pressure and time of reaction were investigated and was studied. High methacrolein conversion of 89% and with high methyl methacrylate selectivity of 98% was attained without the use of any external additives. The synergistic effect between the surface Au NPs and  $La_2O_3$  nanorods plays an important role towards the activity of the catalyst.

## Ultrathin Membranes and 3D Nanoarchitectures of Hollow Tetrapodal Structures Based on GaN and $\beta$ - $Ga_2O_3$ for Multifunctional Application

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## Abstract

We report on development of large-sized ultrathin GaN single crystalline membranes and of 3D nanoarchitectures based on GaN hollow microtetrapods with nanoscopic thin walls. It is shown that memristive networks consisting of GaN ultrathin membranes exhibit learning mechanisms such as habituation and dishabituation followed by storage of the response to a certain electrical stimulus, while the 3D nanoarchitecture based on GaN hollow microtetrapods (called aero-GaN) represents the first artificial material exhibiting dual hydrophobic-hydrophilic behaviour (see <https://physicsworld.com/a/hydrophobic-or-hydrophilic-aero-gallium-nitride-is-both/>). The GaN hollow microtetrapods are shown to self-organize when interacting with water, forming self-healing waterproof rafts and self-propelled liquid marbles promising for microfluidic applications. Heat treatment allows one to reach effective oxidation of GaN and thus to fabricate nanocrystalline ultrathin  $\beta$ - $Ga_2O_3$  membranes and 3D nanoarchitectures based on  $Ga_2O_3$  hollow microtetrapods (called aero- $Ga_2O_3$ ). The aero-GaN exhibits shielding capabilities against electromagnetic radiation in both GHz and THz regions, while aero- $Ga_2O_3$  shows high transparency at GHz and THz frequencies. The support from the European Commission under Grant #810652 “NanoMedTwin” is acknowledged.

## Designing TiAl-based Nanocomposite Through Semi-coherent Nanoprecipitates

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## Abstract

TiAl intermetallics are widely used in engines as high temperature lightweight structural materials. Dispersion-strengthening, an effective mean to further improve the high temperature performance of metals, is failed to implement into TiAl intermetallics. Here, we fabricate a TiAl naocomposites with fully-lamellar microstructures and homogeneously dispersed  $Ti_2AlC$  nanoprecipitates via spark plasma sintering. The composites consisted of semi-coherent interfaces among  $\gamma$ -TiAl/ $Ti_2AlC$  precipitates /  $\alpha_2$ - $Ti_3Al$ , in addition to continuous polysynthetically nanotwins (PST). Strong pinning effect of  $Ti_2AlC$  as well as strain-induced nanoscale  $TiCr_2$  precipitation enhance the operation temperature of TiAl nanocomposites more than 50 . Strain induced complex interfacial interactions promoted dynamic recrystallization, which further improve the ductility. In-situ  $Ti_2AlC$  precipitates serve as oxygen

diffusion barrier during isothermal oxidization, and significantly drop down the mass gain of the TiAl nanocomposites. In-situ Ti<sub>2</sub>AlC reinforced TiAl-based nanocomposites has excellent combination of high temperature strength and oxidation resistance, is a promising light weight structural materials for potential application in automotive and aerospace industries.

## Surface-confined Synthesis of Ultrafine Pt-Rare Earth Nanoalloys on N-Functionalized Supports

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<sup>d</sup>Chemistry and Chemical Engineering of Guangdong Laboratory, China

### Abstract

Controllable preparation of rare earth-containing nanoalloys is particularly challenging because of the ultralow standard reduction potential of rare earth metals. Herein, we demonstrate a conceptually new surface-confinement strategy to controllably synthesize ultrafine Pt-rare earth nanoalloys on a variety of N functionalized supports. By virtue of this method, ultrafine Pt-La, Pt-Y and Pt-Dy nanoalloys are prepared on various N functionalized supports like carbon, HY zeolite and Al<sub>2</sub>O<sub>3</sub>. The formation mechanism is carefully explored: (i) it is found that through the N-metal coordination on the surface of the N functionalized supports, metal cations of precursors are homogeneously atomically dispersed thereon, which largely promotes uniform nucleation and growth of the Pt-rare earth nanoalloys upon hydrogen reduction. (ii) in another regard, particle growth is confined to a narrow region via N-controlled metal transfer, hence favoring formation of ultrafine Pt-rare earth nanoalloys. Remarkably, the Pt-La nanoalloys supported on N functionalized HY zeolite display excellent catalytic properties for propane oxidation reaction. Our method is expected to open up new opportunities to controllable synthesis of highly efficient rare earth-containing nanocatalysts.

## Environmental and Performance Assessment of Hydrophobic and Flame-retardant Cotton Fabrics Modified with Functional Integrated Graphene

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### Abstract

There is a conflict between enhancing the functionality of products and reducing the environmental impact of manufacturing in the materials industry. Using green chemicals or adopting cleaner production processes can help overcome this conflict. However, researchers usually neglect the substitution effect when selecting green technology, namely, that investing more in chemical development decreases the resources used in cleaner process techniques. This study demonstrated this substitution effect in the modification of cotton fabrics. We fabricated hydrophobic and flame-retardant cotton fabrics with functional integrated graphene. It was found that these fabrics can be prepared in one step. As seen from an environmental assessment, applying functional integrated graphene can decrease the time required, reduce the energy consumption, and reduce the wastewater discharge. Based on the hydrophobicity-flame retardancy quadrant, we found that functional integrated graphene can improve the compatibility of different functionalities. On the other hand, compared to the use of commercial finishing agents, using functional integrated

graphene can reduce organic discharge by up to 92%. This study demonstrates that using green chemicals can reduce pollution discharge and result in a cleaner production process. This study also provided atom economic ideas for green modification of cellulosic materials.

## **Doping Engineering of Single-walled Carbon Nanotubes by Nitrogen Compounds Using Basicity and Alignment**

**Karolina Z. Milowska<sup>a,b,c</sup>, Bogumiła Kumanek<sup>d</sup>, Łukasz Przypis<sup>d</sup>, Grzegorz Stando<sup>d</sup>, Karolina Matuszek<sup>e</sup>, Douglas MacFarlane<sup>e</sup>, Mike C. Payne<sup>a</sup> and Dawid Janas<sup>d</sup>**

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<sup>b</sup>*CIC nanoGUNE, Spain*

<sup>c</sup>*Ikerbasque, Basque Foundation for Science, Spain*

<sup>d</sup>*Department of Organic Chemistry, Bioorganic Chemistry and Biotechnology, Silesian University of Technology, Poland*

<sup>e</sup>*Monash University, School of Chemistry, Australia*

### **Abstract**

Charge transport properties in single-walled carbon nanotubes (SWCNTs) can be significantly modified through doping, tuning their electrical and thermoelectric properties. In this study, we used more than 40 nitrogen-bearing compounds as dopants and determined their impact on the material's electrical conductivity. The application of nitrogen compounds of diverse structures and electronic configurations enabled us to determine how the dopant nature affects the SWCNTs. The results reveal that the impact of these dopants can often be anticipated by considering their Hammett's constants and pK<sub>a</sub> values. Furthermore, the empirical observations supported by first-principles calculations indicate that the doping level can be tuned not only by changing the type and the concentration of dopants but also by varying the orientation of nitrogen compounds around SWCNTs. In particular, we will show how induce the transition from n- to p-type doping by only changing the temperature of octylamine-doped SWCNT films.

## **Superficial Nanograins Obtained by Cold Rolling with Rough Rolls and Annealing. Modeling and Experimental Results**

**Carlos Camurri\* and Yasmin Maril**

*University of Concepcion, Chile*

### **Abstract**

A new process is developed to obtain superficial nanograins in largest areas of metallic materials, consisting on a cold rolling with rough rolls- roughness height between 0.1 and 1 mm- followed by an annealing at low temperatures.

The process is simulated by FEM analysis, obtaining good correlations with the experimental rolling force and the average size of the superficial nanograins, of 200-300 nm for the case of a 316L stainless steel.

Also, the steel surface as higher nano hardness and wear resistance compared with those obtained under the same conditions but rolled with smooth rolls.

## **Reaction Conditions and Aqueous Washing Process: Implications for Graphene Oxide Production**

**Camila Mora<sup>a\*</sup>, Toribio Figueroa<sup>b</sup> and Antonio Buljan<sup>c</sup>**

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<sup>c</sup>University of Concepcion, Department of Physicochemistry, Chile

## Abstract

The oxidation reaction of graphite with potassium permanganate in sulfuric acid has been widely discussed in the literature; however, its application on an industrial scale lacks a detailed methodological review that describes the interaction of variations in reaction conditions. This long-range study reviews the reaction conditions in addition to analyzing in detail the sample washing process; the objective is to understand the process of oxygen transfer to graphite sheets to adapt the reaction conditions according to the graphene oxide applications. Results of the systematic variations of the reaction conditions indicate that longer reaction times favor solubility because of a greater presence of C-O and O-C=O groups, the proportion of permanganate determines the homogeneity in the distribution of oxygenated groups, and it is demonstrated that the reaction is efficient at room temperature, avoiding damage to the sp<sup>2</sup> structure of the carbon. Washing analysis, it has been determined that it is the water that transfers oxygen to the graphite during the washing process. This result indicates the importance of describing the washing process as part of the reaction itself and allows us to more precisely define the amount of water to use according to the needs of our product. Thus, from both results, the graphite oxidation process has been redefined considering the washing process, describing three stages: stage 1, primary oxidation; stage 2, ion removal; stage 3, main oxidation, and sheet separation. The results of this study allow one to define the reaction conditions suitable for the use of the GO prepared.

## Thermoelectricity in Hybrid 2D Materials

Taher Ghomian

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### Abstract

Much of the research in thermoelectric devices has been dedicated to nanostructured materials. Quantum confinement phenomena in nanomaterials can improve the Seebeck coefficient, and surface and interface effects in nanomaterials can efficiently scatter phonons leading to much lower thermal conductivity as maintaining electrical conductivity. In the hybrid nanostructured systems, organic linkers on the surface of the nanoparticles significantly affect the thermoelectric performance of the system by limiting phonon mode propagation through the entire lattice, playing an essential role in the electrical conductivity of the system, and determining the Seebeck coefficient. Moreover, for real applications, a large system must be implemented. The Seebeck coefficient of a large hybrid system depends not only on the Seebeck coefficient of the individual molecular junctions but also on the interactions of the components in the system.

This presentation concentrates on the effect of the organic linkers and system dimensionality on the thermoelectric performance of 2D hybrid systems. In particular, the effects of destructive quantum interference in molecular junctions and the lattice dimensionality on the Seebeck coefficient of a large system of molecule/Au nanoparticle 2D arrays will be discussed.

## Visualizing Atomically layered Magnetism in CrSBr

Daniel J. Rizzo<sup>a\*</sup>, Alexander S. McLeod<sup>a</sup>, Caitlin Carnahan<sup>b</sup>, Evan J. Telford<sup>c</sup>, Avalon H. Dismukes<sup>c</sup>, Ren A. Wiscons<sup>c</sup>, Yanan Dong<sup>a</sup>, Colin Nuckolls<sup>c</sup>, Cory R. Dean<sup>a</sup>, Abhay N. Pasupathy<sup>a</sup>, Xavier Roy<sup>c</sup>, Di Xiao<sup>d</sup> and D.N. Basov<sup>a</sup>

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## Abstract

Layered magnetic materials have recently garnered considerable interest as platforms for realizing tunable magnetic devices and studying fundamental two-dimensional (2D) magnetic properties. A growing body of research on chromium-based van der Waals (vdW) materials demonstrates the existence of magnetism in 2D films down to single atomic layers. Among these, CrSBr has emerged as an air-stable layered antiferromagnetic (AFM) semiconductor with a high transition temperature ( $T_N \approx 132$  K) and gate-tunable magnetic ordering. However, real-space visualization and temperature evolution of magnetic domains in CrSBr remains unexplored, and requires a sensitive local probe. To achieve this, we conducted a variable-temperature magnetic force microscopy (MFM) study under ultrahigh vacuum (UHV) conditions, revealing incipient magnetism well above  $T_N$  associated with the onset of in-plane magnetic correlations which eventually give way to layer-dependent magnetization in the low-temperature AFM phase ( $T < T_N$ ). In addition, we observe temperature-dependent magnetic susceptibility and switching with a high degree of spatial inhomogeneity arising, in part, from the parity of the underlying layer number. Our work demonstrates that MFM functions as a sensitive local probe of magnetic susceptibility in the 2D limit.

## Effect of K Doping on Structural, Optical and Dielectric Properties of Tin Selenide Prepared by Hydrothermal Method

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## Abstract

In this study, the effect of potassium doping on the Structural, Optical and dielectric properties (temperatures between 323K -523K and frequencies from 100Hz to 12 MHz) in Tin Selenide (SnSe) has been investigated. The Potassium doped SnSe ( $K_xSn_{1-x}Se$  with  $x= 0-20$  mol %) polycrystals were prepared by hydrothermal method. The phases of the synthesized samples was confirmed to be orthorhombic single-phase as obtained by X-Ray Diffraction. The average crystallite size obtained from Debye-Scherrer formula showed a decrease with increase of potassium (K) concentration. A Plate-like morphology was obtained for all  $K_xSn_{1-x}Se$  samples as revealed by Scanning Electron Microscope. Transmission Electron Microscope studies at high resolution exhibited plate-like-morphology connected with small nanorods for the  $K_{0.20}Sn_{0.80}Se$  sample. The bandgap values were found to be decreased with increase in K concentration.  $K_{0.20}Sn_{0.80}Se$  sample exhibited giant value of dielectric constant and ac conductivity at room temperature and high temperature. Correlated Barrier Hopping (CBH) is the probable mechanism for the transport of charge carriers in the conduction phenomenon. Electrical modulus studies revealed a non-Debye type dielectric relaxation phenomenon. The results of dielectric studies identify the application of K-doped SnSe in frequency-related and capacitive storage devices.

## Young Researcher Presentations

### Moiré Regulated Friction in Low-Angle Twisted Bilayer Graphene

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## Abstract

We demonstrate moiré-regulated stick-slip friction of a nanoscale silicon probe sliding on low-angle twisted bilayer

graphene (tBLG) using fully atomistic nonequilibrium molecular dynamics simulations with state-of-art force fields. The moiré-level regulation is found to be significant only when the probe sliding over the corners of moiré superlattices (i.e., it's the AA-stacking region). Otherwise, only atomic stick-slip events can be observed. Simulation results show that the periodicity of moiré-scale stick-slip phenomenon depends on the twist angle of tBLG and its peak force increases almost linearly with the applied normal load. Further theoretical analysis revealed that the elastic distortions of moiré superlattices is the main origin of moiré-regulated stick-slip friction. Our findings provide new insights to understand the critical role of moiré superlattice on frictional properties of vdW heterostructures and open an avenue for rational design of vdW devices with controllable tribological properties.

## Core-shell Upconversion Nanoparticles Synthesis and Surface Modifications with Polymers Using PET-RAFT Polymerization

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### Abstract

The unique feature of lanthanide doped upconversion nanoparticles (UCNPs), is to absorb near infrared (NIR, low energy) radiations and emit light of higher energy (UV and visible light), thereby displaying upconversion (UC) mechanism. Further, these UCNPs have been reported to display excellent photo-stability, narrow emission peaks, deep tissue penetration, and low biological toxicity, which makes them potential candidates for biological luminescent labels. Surface modification with appropriate functionalities is a major requirement to make them water dispersible as well as bio-compatible. It is to be noted that the surface of these UCNPs could easily be functionalized by polymers using “Grafting from” approach via photoinduced electron/energy transfer – reversible addition fragmentation chain transfer (PET-RAFT) polymerization, which is considered as sustainable and greener approach, using light as external stimuli. Herein, we have synthesized NaYF<sub>4</sub> based Lanthanide (Er<sup>+3</sup>) doped UCNPs system, which was further coated by organoalkoxysilane based RAFT agent. The resulting core@shell architecture was further modified using variety of polymers which were anchored using “grafting from” approach. The grafting of polymers on the UCNPs surface was performed via PET-RAFT polymerization using external blue light ( $\lambda$ -540nm) as stimuli in the presence of organic dye acting as photocatalyst, under room temperature conditions. The modified UCNPs so obtained were isolated and their morphological, structural as well as thermal characterizations were performed to validate their core@shell@shell framework. In addition, their Photoluminescence measurements were performed using 980 nm laser source and the developed core@shell@shell framework of UCNPs will be analyzed for its cellular uptake and cytotoxicity.

## Electrodeposited Nickel–graphene Nanocomposite Coating: Influence of Pulsed Current Density on Microstructure and Wear Resistance for Friction Control Applications

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<sup>c</sup>*Department of Engineering, University of Tuscia, Italy*

### Abstract

Protective and wear-resistant coatings are increasingly being used to obtain the best combination of functional properties in order to reduce friction and wear-related mechanical failures. Graphene-based nanomaterials, such as graphene oxide (GO), are highly suitable as reinforcing element in many composites. This paper investigates the influence of pulsed current density on microstructure and wear resistance of functionalized-GO reinforced nickel coatings (Ni/fnGO). The composite coatings were produced via pulsed co-electrodeposition and compared to the relevant Ni-coating. The morphology of the coatings was investigated using a 3D Surface Profiling System. Dry sliding wear tests were executed in linear (reciprocating) mode on the coating surface to evaluate the tribological

performance. The deposits microstructure and wear mechanisms were studied through Scanning Electron Microscopy (SEM) observations, while the cohesion and the adhesion of the coatings via scratch tests. Based on the experimental results, the Ni/fnGO coatings reduce the friction coefficient in dry sliding against steel. The composite coating at low current density achieves the higher tribological performance, (18% ca reduction of the friction coefficient at 10,000 cycles), and the improvement of the friction coefficient is inversely related to the current density. In fact, SEM and morphological analysis indicate a reinforcement decrease into the metal matrix as the current density increases. The authors propose that low current density favor the co-deposition of functionalized-GO, mainly due to the inherent probabilistic nature of the process, reducing this way the deposition rate of the metal.

## Replacement of Pd with Magnetically Separable Hierarchical NiZn Alloy Nanoparticles for Suzuki-Miyaura Coupling Reaction

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### Abstract

C-C bond forming Suzuki coupling reaction has been extensively studied and investigated over the years using Pd based catalysts. The reaction is employed in the synthesis of many industrially significant chemicals, pharmaceuticals and agrochemicals, so a noble metal free protocol will be appreciably economical for biaryl production. Transition metal based bimetallic alloy nanoparticles can serve the best purpose because of its ability to display higher catalytic activity than noble monometallic counterparts. Alloying is known to mankind since Bronze Age when combining two metals gave a material much stronger, possessing high ductility and malleability than the corresponding individual atoms. Not just the physical properties but the chemical properties also get enhanced due to alloying and therefore it is emerging as a significant topic in the area of nanocatalysis. The liveness offered by nanoalloys in fabricating materials with desired and controllable properties and structure in the nanoscale has attracted attention of the material science community. We have hence designed inexpensive NiZn nanoalloy and characterized the same by various analytical techniques such as PXRD, SEM, HR-TEM, EDS mapping and XPS and confirmed the formation of hexagonal homogenous alloy with the constituent elements in the metallic state. Our designed NiZn nanoalloy showed appreciable activity in the biaryl synthesis via Suzuki-Miyaura cross coupling between arylboronic acid and haloarene. The presence of Ni makes the nanoalloy a weak ferromagnetic substance and hence establishing it as an effective magnetically recoverable catalyst.

## Multifunctional Starch/Graphene Oxide/Fe<sub>3</sub>O<sub>4</sub> Nanocomposites with Multiple Stimuli Responsive Properties

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<sup>b</sup>*School of Chemistry and Physics, Faculty of Science, Queensland University of Technology, Australia*

### Abstract

Smart actuators that can be triggered by an external stimulus such as moisture, light, electricity, pH, and magnetic fields have attracted enormous research interest due to their cutting-edge applications in soft robots, smart switches, wearable electronics, nanogenerators, and artificial muscles. However, the traditional soft actuators are mainly limited to a single actuation mode and demand expensive and sophisticated manufacturing methods that use nonrenewable or toxic materials. Moreover, weak mechanical properties, limited cyclic performance, and poor stimuli response still present challenges for practical application. In this study, a novel multiple stimuli responsive soft actuator is fabricated using tapioca starch (a water-soluble natural polymer), graphene oxide, and magnetic Fe<sub>3</sub>O<sub>4</sub> particles via a water evaporation-induced self-assembly method. The resulting actuator is sensitive to three stimuli: moisture, UV light, and magnetic field, owing to the brick-and-mortar like assembly of graphene oxide and starch polymer, and homogeneous dispersion of Fe<sub>3</sub>O<sub>4</sub> particles within the polymer matrix. The tensile strength and toughness of the

actuator are  $59.5 \pm 1.5$  MPa and  $0.95 \pm 0.04$  MJ/m<sup>3</sup>, respectively. To demonstrate the potential applications, this actuator has been successfully utilized as smart grippers, biomimetic structures, and smart curtains.

## Dual-mode Surface-enhanced Raman Scattering Sensors Assembled from Graphene Plasmonic Nanoresonator on Photoactive SOI

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<sup>b</sup>Materials Science and Technology Division, Los Alamos National Laboratory, USA

### Abstract

Surface-enhanced Raman scattering (SERS) has been explored and acts as a practical analytical detection approach. However, constructing highly sensitive SERS substrates usually involves expensive materials and tedious preparation processes, and SERS substrates often cannot be reused. Herein, direct hetero-integration of three-dimensional graphene (3D-graphene) with silicon-on-insulator (SOI) substrate can be utilized as a highly stable, ultra-sensitive, low cost and reusable SERS substrates through plasma-assisted chemical vapor deposition (PACVD). The novel nanocavity construction of the 3D-graphene combines with the optical cavity system of the SOI to improve the interaction between the incident light and 3D-graphene, which is a model for doubly-reinforced Raman scattering. These properties enhance electronic interactions between 3D-graphene, target molecules, and SOI substrates, thereon improving chemical/charge transfer effects in heterojunctions. The as-designed 3D-graphene/SOI heterojunction have detection limits of  $10^{-10}$  M for rhodamine B (RB) and rhodamine 6G (R6G), and detection limits for crystalline violet (CRV) is  $10^{-8}$  M. Besides, Our study confirms the efficient carrier transfer mechanism in the 3D-graphene/SOI heterojunction and enhances the chemical/charge transfer mechanism of SERS by double-enhanced high-light absorption. In addition, erythrosine B (EB) and carmine, considered a harmful pigment additive in fruit-flavored beverages, was selected as the detection target with a detection limit of about  $10^{-9}$  M and  $10^{-8}$  M, suggesting that 3D-graphene/SOI heterojunction-based SERS can be applied in the food safety field.

## Broccoli-liked Silver Phosphate Nanoparticles Supported on Green Nanofiber Membrane for Visible-light Driven Photodegradation Towards Water Pollutants

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### Abstract

In view of the practical application, it is imperative to develop efficient, exercisable, and visible-light driven water pollution treatment materials. Herein, a high-efficiency green photocatalytic membrane for water pollution treatment is proposed and fabricated conveniently. Firstly, silver phosphate ( $\text{Ag}_3\text{PO}_4$ ) nanoparticles with controlled morphology were prepared by simple liquid-phase precipitation method, and then a hierarchical structured  $\text{Ag}_3\text{PO}_4$ @polylactic acid (PLA) composite nanofiber membrane was prepared by electrospinning. Using electrospun PLA nanofiber membrane as a carrier of photocatalysts can significantly improve the dispersion of  $\text{Ag}_3\text{PO}_4$  nanoparticles, and increase the contact probability with pollutants and photocatalytic activity. The prepared  $\text{PLA}@Ag_3PO_4$  composite membrane was used to degrade methylene blue (MB) and tetracycline hydrochloride (TC) under visible light irradiation. The results showed that the removal ratio of pollutants on  $\text{Ag}_3\text{PO}_4$ @PLA composite nanofiber membrane was 94.0% for MB and 82.0% for TC, demonstrating an outstanding photocatalytic activity of composite membrane. Moreover, the PLA nanofiber membrane is a self-supported and biodegradable matrix. After five cycles, it can still achieve 88.0% of the initial photocatalytic degradation rate towards MB, showing excellent recyclability. Thus, this composite nanofiber membrane is a high-efficiency and environmental-friendly visible-light driven water pollution treatment material that could be used in real applications.

## Nanostructured (Sn,Ti,Nb)<sub>x</sub>O<sub>2</sub> Solid Solution for Gas Sensing Applications

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### Abstract

Emerging nanotechnologies improved solid-state sensors capabilities and enabled the use of semiconducting metal oxides-based gas sensors for new and increasingly demanding applications. However, further research on sensing materials is still needed to increase the sensitivity, selectivity and stability of such sensors.

Nanostructured metal-oxide solid solutions represent a valuable approach for tuning the sensing properties by modifying their composition, morphology, and structure. For example, tin and titanium dioxides (SnO<sub>2</sub> and TiO<sub>2</sub>) would easily form solid solutions since they can exhibit a rutile type structure where octahedrally coordinated Ti<sup>4+</sup> and Sn<sup>4+</sup> have similar ionic radii. Such solid solution combines the positive qualities of the singles oxides, e.g., high sensitivity towards reducing gases and low influence by humidity.

Such solid solution was empowered by addition of Nb, which – according to earlier studies on titania films – was expected to inhibit grain growth at high temperature, to reduce the film resistance and to impact the sensor selectivity and sensitivity. Nanostructured (Sn,Ti,Nb)<sub>x</sub>O<sub>2</sub> powders were synthetized through co-precipitation by keeping the Sn/Ti proportion constant at the optimal value for sensing performance, while changing Nb concentrations and calcination temperature. Powder compositions, structures and morphologies were investigated by different techniques. The electrical characterization of the sensors based on nanostructured (Sn,Ti,Nb)<sub>x</sub>O<sub>2</sub> showed that the niobium concentration and the heating treatment of powders are fundamental parameters to optimise the sensing characteristics of a sensor.

## Session: Future Materials: Characterization, Theory and Design

### Featured Presentations

#### Design of the Microwave Propagation Parameters in Magnetic Fluids

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<sup>b</sup>Trinity College, Department of Electronic and Electrical Engineering, Dublin, Ireland

### Abstract

Magnetic fluids (or ferrofluids) belong to the class of functional materials, with both fluid properties and soft magnetic material characteristics. They can be involved in various microwave applications (such as: frequency selective surfaces, liquid antenna, microstrip filter, patch antenna, magnetically controlled elements of circuits or microwave shielding with ferrofluidic meta-skin).

The talk presents an example of the design of the electromagnetic wave propagation parameters in ferrofluids, based on the theoretical description of the frequency and static magnetic field dependencies of the complex magnetic permeability and of the complex dielectric permittivity of ferrofluids.

The theoretical results are compared with experimental results obtained for a ferrofluid with magnetite particles dispersed in kerosene, for which measurements were made by the coaxial line method (short /open), over the frequency range from 0.1 GHz to 6 GHz.

## Materials Beyond Copper for CO<sub>2</sub> Reduction Reaction

Samira Siahrostami

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### Abstract

Copper-based catalysts are currently being increasingly examined as the most efficient catalysts for CO<sub>2</sub> reduction reaction (CO<sub>2</sub>RR) to valuable hydrocarbons such as ethylene and ethanol. However, they suffer from low activity and selectivity. We use high-throughput DFT calculations to search a wide range of materials space and expedite discovery of more efficient catalyst materials beyond copper for CO<sub>2</sub>RR and scale-up the use of the catalysts in electrochemical reactors to enable meaningful conversion. In this talk, I will discuss the use of robust high-throughput DFT calculations to screen a massive library of non-conventional classes of materials such as perovskites and transition metal nitrides and the insight we can obtain from them.

## Creation and Mechanical Simulation of Graded Gyroid Structures

Leonie Wallat<sup>a,b\*</sup>, Patrick Altschuh<sup>b,c</sup>, Martin Reder<sup>b</sup>, Britta Nestler<sup>b,c</sup> and Frank Poehler<sup>a\*</sup>

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*<sup>c</sup>Institute for Applied Materials – Microstructure Modelling and Simulation, Karlsruhe Institute of Technology, Germany*

### Abstract

Triply periodic minimal surface (TPMS) structures are mathematically definable three-dimensional cell structures. These structures are attracting attention in a wide variety of research areas, from heat exchangers (because of their high surface-to-volume ratio) to possible bone structures (because of their similarity to nature). The best-known structures are Schwartz Diamond, Schwartz Primitive and Gyroid. The focus of this work is on the gyroid structure.

Unicellular sheet-based gyroid structures with different porosities and gradients (linear, quadratic and constant) are compared by mechanical simulations in the linear deformation regime. The parameters are converted into dimensionless quantities, which allows material-independent statements. Thus, only statements about the structural geometry can be made. The results of the mechanical simulation are then compared with experimental results.

## Density-functional Simulations for Novel Materials

Wei Wu

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### Abstract

Density-functional theory is an immensely powerful tool to model materials. Here we demonstrate the materials modelling by using density functional theory for a few types of new materials for a wide range of applications including semiconductors, light emitting diodes, transparent conductors, and spin-chain compounds for toroidal moments. Recently we have computed the water adhesion on silicene quantum dots by using hybrid-exchange density functional theory and found the tilted structure of water/ice, which could have a technological implication for anti-icing. DMAC-based molecules are important components for the application in light emitting diodes. We have also used time dependent density functional theory to compute the absorption and emission spectra of four

typical DMAC TADF molecules. From this we have found the functional need to be improved further even beyond range-separated hybrid density functional, to have a comprehensive agreement with the experiment. Moreover, we have used density functional theory to study the electronic structure of transparent conducting oxides. By doping different types of elements, we can control the electronic states both for the n- and p-type. Our theoretical findings have been supported by recent experimental results. Moreover, we have combined density-functional theory + U and spin-orbit interaction to compute the electronic structure and magnetic properties of sulphide compound newly synthesized under extreme condition,  $\text{Ba}_6\text{Cr}_2\text{S}_{10}$ . In this compound, the quasi-one-dimensional spin chains are dominant on the magnetic properties. Our calculations have implied toroidal moments, which could have important applications for future information storage, could sustain in this material<sup>4</sup>.

## High Entropy Defect Formation for Fast Hydride Conduction

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### Abstract

A high ionic conductivity is usually achieved due to low activation energy, with values of the pre-exponential factor located in the typical range,  $10^4$ - $10^7$  S cm<sup>-1</sup> K. The unique exception to this rule is novel H<sup>-</sup> conductor,  $\text{LaH}_{2.5}\text{O}_{0.25}$ , for which the record-high H<sup>-</sup> conductivity at intermediate temperature is due to anomalously large pre-exponential factor  $7.8 \times 10^{11}$  S cm<sup>-1</sup> K, whereas the activation energy is high (1.3 eV). In this work, we developed DFT-based neural-network-potential for large-scale molecular dynamics (MD) simulation of  $\text{LaH}_{2.5}\text{O}_{0.25}$ , which allowed us to identify the unique H<sup>-</sup> diffusion mechanism in  $\text{LaH}_{2.5}\text{O}_{0.25}$ . We found that the stoichiometric vacancies facilitate 3H<sup>-</sup> ring-like rotations, that result only in short-range H<sup>-</sup> migration and keep the stoichiometric vacancies immobile. At the same time, the long-range H<sup>-</sup> diffusion is due to formation and migration of the mobile vacancies. The mobile vacancy formation gives rise to an extremely large entropy leading to the large pre-exponential factor. A design concept for faster H<sup>-</sup> conductor is proposed based on the findings.

## Advantages of Low-voltage Scanning Electron Microscopy in Optimizing the Properties of the Polymer-Nanoclay Composites

Alaa Madhloom Almansoori

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### Abstract

Field-Emission Gun Scanning Electron Microscopes such as the NovaSEM are a powerful tool in nanocomposites studies because they provide images with high resolution up to few nanometers at a high magnification. An electron beam with low loading energy (2.2 KeV) was used to reduced specimen surface charging and damage. In addition, two different detectors were used for imaging the samples; a Through-lens-detector (TLD) for secondary electron imaging at low magnification and concentric back scatter detector (CBS) using back-scattered electrons to obtain high magnification images. CBS was found the most valuable tool for the challenging task of studying Polymers/clay interfaces. CBS in conjunction with beam deceleration is used to map nanoclay distribution on polymer particles.

In this study, a polymer-nanoclay composite based on polyamide 12 as a matrix were prepared using dry mechanical mixing before fabricating into tensile test samples using laser sintering. Nanoclay powders were treated using plasma treatment technique to reduce the unwanted agglomeration of nanoclay particles on polymer particles. The thermomechanical tests showed an improvement in the properties of the resulting composites as stated in our previous works. The reasons behind this improving can be understood through the SEM imaging.

Low Voltage-SEM CBS imaging has proved as a very powerful technique in optimizing the clay-nanocomposites with respect to mechanical properties, as it allows to assess clay dispersion without the need for Transmission electron microscopy. Thus, the use of air plasma etching of the clay prior to composite preparation succeeded in avoiding the large clay accumulations as demonstrated by SEM images.

## Design Transition-metal-encapsulated Boron Nanotubes to Boost Efficient Nitrogen Fixation by First-Principle Calculations

Yanlu Li\* and Changhui Liu

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### Abstract

Borophene possesses outstanding properties and demonstrates great application potential in catalysis. However, the lack of a controllable strategy for regulating the electronic structures of borophene limits the exploration of this material. Herein, taking advantage of the synergistic effect between metals and boron nanotubes (BNT), we report a core-shell structure that encapsulates early transition-metal nanowires into BNT (TMs@BNT) to improve the inherent electronic structures of borophene for an efficient electrochemical nitrogen reduction reaction (eNRR). These filled BNT with disconnected  $\pi$  conjugation and vacant boron (B)  $p_z$  orbitals enable the regulation of electronic states of B atoms in spatial extent and occupancy that has a great effect on the adsorption strength of intermediates. Using first-principles calculations, we demonstrate that the  $^*N_2H$  adsorption energy is strongly correlated with the distribution of 2p states and charge of B atoms. We utilize the coupling of the d 2p states between B atoms and metals to obtain a quantitative explanation for synergistic effects. Finally, two candidates Mo@BNT and W@BNT are screened, benefiting from their high eNRR activity (limiting potentials of -0.75 and -0.77 V) and high selectivity. This work constructs a bridge between electronic structures and activity trends and paves the way for future eNRR studies.

## Large Transverse and Longitudinal Magneto-Thermoelectric Effect in Polycrystalline Nodal-line Semimetal $Mg_3Bi_2$

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<sup>b</sup>Department of Physics and Shenzhen Institute for Quantum Science & Engineering, Southern University of Science and Technology, China

### Abstract

Topological semimetals provide new opportunities for exploring novel thermoelectric phenomena, owing to their exotic and nontrivial electronic structure topology around the Fermi surface. Recently, we reported on the discovery of large transverse and longitudinal magneto-thermoelectric (MTE) effects in  $Mg_3Bi_2$  in *Advanced Materials* (2022, 34, 2200931). The corresponding paper is high-lighted in Wiley-VCH Hot Topic: Magnetic Materials.  $Mg_3Bi_2$  sample was predicted to be a type-II nodal-line semimetal in the absence of spin-orbit coupling (SOC). We find the maximum transverse power factor of  $2182 \mu Wm^{-1}K^{-2}$  at 13.5 K and 6 Tesla, and longitudinal power factor of  $3043 \mu Wm^{-1}K^{-2}$  in  $Mg_3Bi_2$ , which is 20 times higher than that in a zero-strength magnetic field and is also comparable to state-of-the-art MTE materials. By compensating the Mg loss in Mg-rich conditions for tuning the carrier concentration close to intrinsic state, the sample fabricated in this study exhibits a large linear non-saturating magnetoresistance (MR) of 940% under a field of 14 Tesla. Using density functional calculations, we attribute the underlying mechanism to the parent linear-dispersed nodal-line electronic structure without SOC and the anisotropic Fermi surface shape with SOC, highlighting the essential role of high carrier mobility and open electron orbits in the moment space. Our work offers a new avenue toward highly efficient MTE materials through defect engineering in polycrystalline topological semimetals.

## Revisiting Carbon Dioxide Adsorption on Porous Carbon from a Perspective of Explainable Machine Learning

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### Abstract

The ever-increasing carbon emission requires the development of carbon capture and storage technology. As one of the most promising approaches, adsorption of CO<sub>2</sub> over porous carbon (PC) has been intensively studied due to the low cost, easy synthesis, and high adsorption capacity. However, further improvement on CO<sub>2</sub> adsorption capacity is hindered by the unclear relationship between each physicochemical property of PC and the adsorption capacity. Recently machine learning (ML) has achieved giant progress in predicting the adsorption capacity based on the physicochemical properties of PC. However, due to the intrinsic “black box” property of ML, the quantitative relationship between each physicochemical property and corresponding adsorption capacity cannot be derived. Herein, Shapley Additive Explanations (SHAP), a powerful visualization tool, was adopted to provide insights into the individual prediction. The results showed that textural property is more important than chemical composition in affecting CO<sub>2</sub> uptake. Meanwhile, both the contribution of each physicochemical property of PC on adsorption and the synergistic effect between chemical compositions are value dependent. This study sheds light on the understanding of CO<sub>2</sub> adsorption mechanism on PC and guides the design of next generation high-performance PC for carbon capture and storage.

## Quasi-Freestanding Bilayer Borophene on Ag (111)

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### Abstract

The lattice structure of monolayer borophene depends sensitively on the substrate yet is metallic independent of the environment. Here, we show that bilayer borophene on Ag(111) shares the same ground state as its freestanding counterpart that becomes semiconducting with an indirect bandgap of 1.13 eV, as evidenced by an extensive structural search based on first-principles calculations. The bilayer structure is composed of two covalently bonded  $\nu_{1/12}$  boron monolayers that are stacked in an AB mode. The interlayer bonds not only localize electronic states that are otherwise metallic in monolayer borophene but also in part decouple the whole bilayer from the substrate, resulting in a quasi-freestanding system. More relevant is that the predicted bilayer model of a global minimum agrees well with recently synthesized bilayer borophene on Ag(111) in terms of lattice constant, topography, and moiré pattern.

## Operando DRIFT for Surface Reactivity Studies on Chemiresistive Gas Sensor

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## Abstract

The increasing demand for precise detection of gaseous molecules towards diverse applications has led to expanding research for high-performance semiconductor-based chemical sensors. In particular, the employment of nanostructured materials in sensing films has stimulated the development of chemiresistive gas sensors, demonstrating that a change of nanostructures morphology leads to a change of active surface area and ultimately to the gas sensor sensitivity. Therefore, it becomes fundamental to deeply investigate the chemical phenomena occurring at the sensing film surfaces while analyzing the connected variations of the electronic structure and sensing characteristics. This correlation has become critical in chemical sensors since it represents the core of the gas-detection mechanism. Among the arsenal of characterization tools available to support mechanistic proposals, Fourier-transform infrared spectroscopy (FTIR) spectroscopy has been known for the investigation of surface chemistry of nanostructured materials. Accordingly, a variety of cells for in situ and operando spectroscopy have been developed for transient catalytic investigations. We designed, fabricated, and validated a new gas sensing system, which can be employed with solid-state gas sensors at operating temperatures up to 650 °C. It is equipped with a precision stage for the alignment of the sample, and it is fully compatible with Harrick Scientific's diffuse reflection optics.

## A Model of the Elastic Energy of a Bifurcated Wafer: A Benchmark of the Analytical Solution vs. the ANSYS Finite Element Analysis

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## Abstract

Bifurcation significantly impacts the warpage in wafers and consequently the yield and reliability of final systems in packages (SiPs). Gaining more insights in its features is crucial in the semiconductor industry and in the specific sector of power electronics. To this end a physical quantity that has not been investigated extensively is the value of the bifurcation energy of a wafer. In this work, an analytical model of the dependence of the bifurcation energy of the substrate on the residual stress has been developed for a metalized wafer. The analytical model has been validated by exploiting Finite Element Analysis (FEA) methods. In the specific, ANSYS® simulation experiments have been designed to determine the substrate energy for the use-case of an 8" silicon 500 µm thick wafer metalized with a 4.5 µm aluminum layer, both in the spherical and bifurcation case. In the simulations, the bifurcation has been induced in the wafer by applying a pair of weak forces acting as perturbations along two perpendicular directions. The applied forces and the energy of the substrate has been assessed within a theoretical framework. The resulting principal curvatures of the wafer have been analyzed according to the bifurcation diagram reported by the theory. Moreover, it is proven that the bifurcation energy is systematically lower with respect to the spherical case as the residual stress increases and has a second order power law predicted by the analytical model. These results can be generalized by diversifying the metal layer and the substrate, as well. The findings of the paper can be extended to other semiconductor substrates such as silicon carbide (SiC).

## Stress Avalanches of Polyethylene Terephthalate Fiber Reinforced Concrete Beams During Flexure

Zhuang Liu<sup>a</sup>, Robert Worley II<sup>a</sup>, Fen Du<sup>b</sup>, Mandar Dewoolkar<sup>a</sup>, Dryver Huston<sup>a</sup> and Ting Tan<sup>a</sup>

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<sup>b</sup>*Vermont Technical College, Burlington, USA*

## Abstract

Stress-time avalanches of recycled Polyethylene Terephthalate (PET) fiber reinforced concrete during flexure were investigated based on high temporal resolution signals in this study. Stress drops were extracted based on measurements collected at 100 kHz and modeled them as avalanches using the mean field model. Two types of avalanches were observed during flexure of PET fiber beams, i.e., small avalanches collapsed on the scaling regime

and large avalanche beyond the regime. The measured stress drop profiles of small avalanches in the scaling regime agreed with predictions from the mean field theory that has been used to model avalanches. It is interesting to observe that when the peak stress was reached after the fracture of bottom concrete, the post-peak avalanche size could exceed the avalanche size at the bottom fracture. Findings from this study could provide essential clues to the understanding of fiber reinforced concrete during bending.

## Ab Initio Calculations for Void Swelling Bias in $\alpha$ and $\delta$ -plutonium

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### Abstract

Void swelling can develop in materials under persistent irradiation when non-equilibrium vacancy and self-interstitial populations migrate under sufficiently asymmetric interaction biases. In conventional metals, the propensity is determined to first approximation by comparing point-defect relaxation strains. We thus present DFT-based calculations of structures and formation energies and volumes of point defects in the  $\alpha$  and the  $\delta$ -phases of plutonium. We discuss pros and cons of various levels of electronic structure theory: spin-polarization, spin-orbit coupling, and orbital polarization. Our results show that lattice defects in  $\delta$ -Pu, in contrast to most fcc metals, have surprisingly small formation volumes. Equally unexpected are the large defect formation volumes found in the low-symmetry  $\alpha$ -Pu phase. Both these unusual properties can be satisfactorily explained from defect-induced spin/orbital moment formation and destruction in the Pu phases. Surprisingly, the point defects in  $\alpha$ -Pu are found to induce far larger transformation of the local electronic structure than in  $\delta$ -Pu. When we use the calculated defect properties to estimate the classic void swelling bias in each of the phases, we find it to be unusually small in  $\delta$ -Pu, but likely much larger in  $\alpha$ -Pu. Hence, swelling rates and mechanisms can diverge dramatically between the different phases of Pu.

## Young Researcher Presentations

### FIB Lamellae Preparation for Atomic-resolution STEM imaging from Ion-beamsensitive Topological Insulator Crystals

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<sup>c</sup>*Electron Microscopy Centre, University of Wollongong, Australia*

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### Abstract

Good specimen quality is a key factor in achieving successful scanning transmission electron microscope analysis. Thin and damage-free specimens are prerequisites for obtaining atomic-resolution imaging. Topological insulator single crystals and thin films in the chalcogenide family such as  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Te}_3$  are sensitive to electron and ion beams. It is, therefore, challenging to prepare a focused ion-beam (FIB) lamella suitable for high-resolution imaging from these topological insulator crystals using standard focused ion-beam instruments. We have developed a modified method to fabricate thin FIB lamellae with minimal ion-beam damage and artifacts. The technique described in the current study enables the reliable preparation of high-quality transmission electron microscope (TEM) specimens necessary for studying ultra-thin surface regions. We have demonstrated that by carefully optimizing the FIB milling parameters at different stages, a modern Ga-FIB is capable of preparing a high-quality

cross-sectional lamella of chalcogenide topological insulators ( $\text{Sb}_2\text{Te}_3$ ) for STEM analysis. These materials are extremely susceptible to amorphization even at a relatively low fluence of Ga ion-beam irradiation. Guided by the Monte Carlo SRIM calculations and past experience, we developed a preparation recipe for  $\text{Sb}_2\text{Te}_3$  lamellae and provided the details for reference.

## Process-structure-property Relationship of Al- $\text{WS}_2$ Composites Processed by Spark Plasma Sintering and Laser Powder Bed Fusion

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### Abstract

Self-lubricating aluminium-based composites reinforced with solid lubricants promise to meet the demand for lightweight materials in green tribological applications. Laser powder-bed fusion (LPBF) is a metal additive manufacturing (AM) method that selectively melts and fuses metal powder using a high-power density laser beam. Due to the tremendous potential of Al-based composites in various sectors, such as the automotive industry, there has been a global interest in studying their properties when coupled with the unmatched capabilities offered by LPBF. Spark plasma sintering (SPS) is a relatively young solid-state sintering technique that compacts powder materials at lower temperatures and shorter duration compared to traditional methods. In this work, laser powder bed fusion (LPBF) was deployed for the in-situ fabrication of Al- $\text{WS}_2$  composites for the first time, elucidating the process-structure-property relationships in comparison to reference spark plasma sintering (SPS) samples. The microstructure evolution of SPS and LPBF parts fabricated by different processing parameters is also studied in depth.

## Reactive Compatibilization of Impact Co-polymer Polypropylene and Organically Modified Mesoporous Silica to Prepare Composites Possessing Enhanced Mechanical Properties

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### Abstract

Mesoporous silica nanoparticles (MSNs) were synthesized and evaluated as nano-fillers in impact co-polymer polypropylene (ICP) in its original form as well as post organic modification. MSNs were prepared via base-catalysed hydrolysis of tetraethyl orthosilicate in water-acetone medium. The post-modification on MSNs was conducted using commercially available silane with terminal unsaturated bond, and by modifying silane precursor by chemical treatment via TEMPO initiated thiol-ene chemistry to incorporate extended alkyl chain with terminal hydroxyl groups. The characterization for all types of mesoporous silica prepared was done using TGA, FT-IR, Solid state NMR, XPS, BET, XRD, FE-SEM, and HR-TEM. Reactive compatibilization approach was used to prepare ICP-MSNs composites using 1, 5 and 10 phr as filler loading and were tested for their thermal (TGA, DSC), morphological (SEM), rheological (Parallel Plate Rheometry) and mechanical properties (Tensile, Flexural, Izod Impact strength, DMA). The thermal stability and nucleation was enhanced by addition of nanofillers with respect to neat ICP. Tensile and flexural strength as well as tensile and flexural modulus were improved significantly, while maintaining its impact strength. Rise in zero-shear rate viscosity in ICP-MSNs composites was revealed via analysis of rheological properties. DMA studies showed higher storage and loss modulus with introduction of MSNs in ICP.

## Refining Phenomena of Basic Oxygen Steel Making Process

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### Abstract

Refining phenomena of basic oxygen steel-making processes are very complex with hazardous features due to simultaneous metal-metal, slag-metal, metal-gas, slag-gas, and various chemical reactions at high temperatures. In this study, mass transfer kinetic-based models transformed into a reactor-based approach for steel-making where the interfaces of the reacting phases are in thermodynamic equilibrium, and a fraction of liquid metal as mass transfer by partial flows were considered of basic oxygen steel-making furnaces (BOF). In this work, three adiabatic and two isothermal reactors have been used, which are interconnected with each other to describe the overall refining phenomena of the basic oxygen steel-making process. The macro programming facility of FactSage™ software has been used to understand the thermochemical and kinetics of the basic oxygen steel-making process. The model predictions in terms of the amount of carbon, silicon removal, and slag formation are in good consistent with plant data.

## Optimization of Hybrid Microwave Reduction Roasting of Low-Grade Iron Ore Using Cow Dung

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### Abstract

The reduction of iron ore using cow dung has introduced a new era because of its contribution to energy and emission reduction. Cow dung (fixed carbon: 9.33%, volatile matter 42.76%) used as the reductant in the reduction roasting of low-grade iron ore (Fe 44.53%) in a hybrid microwave furnace with a frequency of 2.45GHz and maximum power of 4kW. The optimum conditions of roasting as determined by taguchi statistical design were found to be temperature: 700°C, time: 5 minute and reductant to feed ratio: 0.4. The magnetic concentrate having 61.2%Fe, 75.9% recovery has a potential to be used for Iron making industry. The magnetization of microwave treated samples were determined using vibrating sample magnetometer (VSM). Characterization studies indicate the formation of magnetite phase under optimum conditions resulting higher total magnetism saturation of the sample. The magnetic susceptibility and saturation magnetization of lean iron ore using cow dung as reductant very effectively enhanced by converting hematite to magnetite at the optimum condition using a controlled hybrid microwave furnace.

## Fabrication of Sm-Co Magnets Using Electrodeposition from Aqueous Solution and R-D Process

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### Abstract

Sm-Co permanent magnets were synthesized by electrodeposition from aqueous solution and a Reduction-Diffusion (R-D) process. Essentially the plating solution contained complex agent, glycine, because there is much difference in reduction potential between Samarium and cobalt. The as-deposited SmCo alloy was incorporation of Co, Sm<sub>2</sub>O<sub>3</sub>, CoO, Sm<sub>2</sub>O<sub>2</sub>S in the film. Sm<sub>2</sub>O<sub>3</sub> and Sm<sub>2</sub>O<sub>2</sub>S are reduced to metallic without reducing agent at great high temperature (>1100 °C). So, in heat treatment with SmCo alloy, Ca granule and NaCl, Sm<sub>2</sub>Co<sub>17</sub> was controlled by reduction and diffusion. Energy dispersive spectroscopy of Scanning electron microscope showed that chemical composition of Sm<sub>2</sub>Co<sub>17</sub> (Sm 10.6at%). X-ray diffraction showed that the plated SmCo alloy was amorphous phase. After R-D process, the SmCo alloy became crystallized Sm<sub>2</sub>Co<sub>17</sub> phase. The magnetic property, magnetic saturation (Ms) and coercivity (Hc), was characterized by magnetic property measurement system (MPMS).

## Comparison of Passivation Ability of $\text{CaOH}^+$ and $\text{OH}^-$ on Steel Bar in Concrete: Experiments and DFT Study

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### Abstract

The passive film formed on steel bar surface in concrete could protect the steel from corrosion, it is of great significance to study the formation mechanism of the passive film in concrete. In this study, the comparison was conducted on the passivation of steel bar induced by  $\text{CaOH}^+$  and  $\text{OH}^-$  in concrete environment. The zeta potential test show that, as the increase of pH values, the zeta potential of iron powder in  $\text{Ca}(\text{OH})_2$  solution becomes more positive, while that in NaOH solution becomes more negative, indicating that the iron surface is mainly adsorbed by cation in simulated concrete pore solution contained  $\text{Ca}(\text{OH})_2$ . The cation was determined as the  $\text{CaOH}^+$  per the hydrolysis component concentration of calcium ion at the pH value of 12-13. Moreover, the electrochemical method were adopted to investigate the passivation behavior of steel bar in NaOH and  $\text{Ca}(\text{OH})_2$  solution. The results show that the stability of passive film formed in  $\text{Ca}(\text{OH})_2$  solution is greater than that in NaOH solution at the same pH value, indicating that the  $\text{CaOH}^+$  has higher passivation ability contrast to  $\text{OH}^-$ . Furthermore, the adsorption mechanism of  $\text{OH}^-$  and  $\text{CaOH}^+$  on Fe (100) surface were investigated by the density functional theory at atomic scale. The results show that the interaction of Fe (100) surface with  $\text{CaOH}^+$  is stronger than  $\text{OH}^-$ . In addition, the adsorption of  $\text{CaOH}^+$  could observably decrease the spin value of iron surface and weaken the interaction between iron surface and  $\text{O}_2$ , thereby promoting the passivation of steel bar.

## Session: Materials for Electronics, Optics And Photonics

### Featured Presentations

## Role of Defects and Interfaces in the Exciton and Charge Carrier Dynamics of Semiconductor Nanocrystal

Renato Bozio<sup>a\*</sup>, Marcello Righetto<sup>b</sup> and Alessandro Minotto<sup>c</sup>

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### Abstract

Exciton interactions and dynamics are the most important factors determining the exceptional photophysical properties of semiconductor quantum dots (QDs). Best performances have been obtained for ingeniously engineered core/shell QDs. We have studied two factors entering in the exciton decay dynamics with adverse effects for the luminescence efficiency: exciton trapping at surface and interface traps, and non-radiative Auger recombination in QDs carrying either net charges or multiple excitons. The effect of charge trapping and accumulation at surfaces was investigated for different core/shell QDs: CdSe/CdS, CdSe/CdZnS, and CdSe/ZnS. An in-depth analysis was carried out through time-resolved PL, PLQY and transient absorption measurement. The photophysics of QDs was successfully and exhaustively described by a kinetic model, comprising both trapping and de-trapping processes. Both shell composition and thickness were found to play a pivotal role in modulating these processes which dictate their efficiency in device applications, namely: the smoothness of interface potential, the surface passivation, and

the nucleation of interface defects. Whenever dealing with core/shell systems, we suggest considering three factors to achieve desired properties. For instance, although a ZnS shell provides an optimal surface passivation, the sharp interface potential and the massive nucleation of interface defects hamper their performances. On the other hand, CdS provides a smooth and defect free interface, unfortunately resulting in a poor surface passivation, which turns out to be sufficient only in case of thick shells.

## Recent Progress of Solution-processed Copper-based p-Channel Thin Film Transistors

Hala. A. Al-Jawhari

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### Abstract

The development of well-performing p-type semiconductors is essential in pushing transparent electronics to the next frontier. Copper oxide ( $\text{Cu}_x\text{O}$ ) is a potentially attractive hole-transport material for such applications because of its native p-type semi-conductivity, abundant availability, non-toxic nature, and low production cost. Solution-based processing methods offer many other advantages for the fabrication of metal oxides, including a high level of control over stoichiometry, microstructure and morphology development, as well as tremendous flexibility in terms of materials and end-use architectures. It seems that the last decade has perceived enormous progress in solution processed p-type semiconductors. This talk will cover current progress of synthesis and deposition of solution-based  $\text{Cu}_x\text{O}$  thin films for the purpose of thin film transistors (TFTs). It will show the rapidly growing effort in this field to utilize low temperature methods, nanoscale patterning and green synthesis. Additionally, the emerging solution-processed TFTs made of nonoxide copper-based semiconductors such as halide and (pseudo) halide materials will be discussed. A comparison between the performances of such devices to that of the vacuum-based TFTs will be presented.

## Thin Films Manifesting Localized Surface Plasmon Resonances, for Sensing and Bioapplications

Joel Borges\*, Diana I. Meira, Patrícia Pereria-Silva, Manuela Proença, Marco S. Rodrigues and Filipe Vaz

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### Abstract

Noble metal nanoparticles (Au, Ag) show remarkable optical responses, because they support Localized Surface Plasmon Resonances (LSPRs). When the nanoparticles are typically one order of magnitude lower than the light wavelength, collective oscillations of conduction band electrons are highly confined, enabling strong extinction bands and electromagnetic-field enhancements. For Au and Ag nanoparticles, the resonance condition is met in the visible range, giving important colour effects since ancient times (e.g., the Lycurgus Cup and stained-glass windows of medieval cathedrals). Plasmonic nanoparticles have received considerable attention over the past few years in many scientific fields. For each application, there are critical issues to be considered once LSPR properties are dependent on the size, shape, interparticle distance, and surrounding dielectric material. Manipulating each one of these morphological characteristics and properties, opens a wide range of possible applications, taking advantage of far-field and near-field phenomena.

In the past few years, different LSPR thin film systems were developed by the authors, namely those composed by Au and Ag nanoparticles, dispersed in dielectric hosts as  $\text{TiO}_2$ ,  $\text{CuO}$ ,  $\text{ZnO}$ , and  $\text{Al}_2\text{O}_3$ . The thin films were prepared with variable composition, by reactive magnetron sputtering followed by heat-treatment at different temperatures to promote the growth of the nanoparticles in different size distributions. The LSPR band was monitored in transmittance mode using a high-resolution LSPR spectroscopy system, to evaluate the performance of the thin films as chemo-, bio- and physical (deformation) sensors. Furthermore, near-field effects are currently being used in biological applications with promising results.

## Acknowledgement

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## Improved Transparency and Electron Lifetime of Quasi-Solid State Iodine-free DSSCs

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<sup>d</sup>University of Bordeaux, CNRS, ISM, France

### Abstract

Among the emerging photovoltaic technologies (PV), dye-sensitized solar cells (DSSCs) are one of the cheapest solutions to expand the PV market in agriculture, glazing, wearable electronics, etc. In this context, this work presents the optimization of iodine-free polysiloxane-based ionic conductors for stable and efficient DSSC with enhanced transparency. DSSCs reaching photovoltaic efficiencies up to 8.3% and improved transparency could be attained. Furthermore, iodine-free DSSCs showed superior electron lifetime and reduced charge recombination as confirmed by open-circuit voltage decay measurements. The Raman spectroscopy confirmed the effective tri-iodide in-situ generation and lack of polyiodide formation, whereas electrochemical measurements proved an increased open circuit voltage for devices containing iodine-free electrolytes.

In this communication, we will discuss the strategies implemented to reach these results by optimizing the electrolytes and the photoanode thickness in terms of aesthetics, performance, and stability.

## Semiconducting Nanonets: A Highly Promising Nanomaterial for Macroscale Functional Devices

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### Abstract

The development of functional devices compatible with standard microelectronic processes is central to the More-than-Moore and Beyond-CMOS electronic fields. Devices based on nanowires (NWs) are very promising, but their integration remains complex and submitted to variability limiting the potential scalability. The field of flexible electronics is another one in which the standard microelectronic industry struggles to propose a solution. Despite tremendous progress, organic materials remain highly sensitive to oxygen and humidity and deteriorate under UV irradiation, thus limiting their long-term operation.

With this presentation, we demonstrate that the semiconducting nanonets, two-dimensional networks of randomly oriented nanowires, provide an easy-to-process single answer to develop flexible electronics and NW based devices. In addition, these materials provide an ideal platform for an in-depth study of the physics of percolation. Based on ZnO and Si nanonets, we will demonstrate the fabrication of reproducible P- and N-type transistors with state-of-the-art performance on both standard and transparent and/or flexible substrates.

A focus will also be placed on the key technological elements necessary for the integration of the semiconducting nanonets to produce stable, reproducible and fault tolerant devices.

We are convinced that semiconducting nanonets have a major role to play in future flexible electronics or sensing applications, not only because of their performance and versatility but also because of their potential to support eco-friendly manufacturing processes.

## **An Environmentally Friendly Methodology to Fabricate Light Emitting Germanium Microbridges**

**Cicek Boztug<sup>a\*</sup>, Buse Unlu<sup>b</sup>, Milad Ghasemi<sup>b,c</sup> and Selcuk Yerci<sup>b,c,d</sup>**

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### **Abstract**

Germanium (Ge) is a promising material platform to realize monolithically integrated laser that could enable the fully integrated infrared systems for a variety of applications ranging from optical communication to biosensing. The pseudo-direct bandgap of Ge can be engineered via the application of tensile strain, where direct bandgap Ge has been reported by several research groups for both uniaxial (in [100] direction) and biaxial (in (100) plane) strain types. In this work, for the first time, we fabricated tensilely strained single crystalline Ge microstructures through liquid phase epitaxy in a CMOS-compatible fashion and record-high strain level, as high as 2.4%, has been demonstrated in the [110] direction. The fabrication of the suspended microstructures on silicon is based on an environmentally friendly, room-temperature operated physical vapor deposition tool, namely sputter, where the deposited amorphous Ge is crystallized after a rapid thermal annealing (RTA) process. RTA both enables crystallization of Ge and converts the capping layer into a stressor. The subsequent photolithography process enables to fabricate suspended Ge microstructures with uniaxial tensile strain along the crystallization direction, where strain is transferred from the underetched stressor into the suspended parts of Ge. The strain enhances as the underetched portion of the stressor is increased as verified through the micro-Raman measurements. The fabricated microstructures demonstrate room-temperature light emission, and the emission both red-shifts and enhances with increasing strain as expected. Furthermore, these experimental observations are verified by 3-dimensional finite element methods calculations.

## **Infrared Metasurface with Tailored Differential Emissivity Response**

**Evangelos Vassos<sup>a\*</sup>, Kai Sun<sup>b</sup>, James Churm<sup>a</sup>, Otto L. Muskens<sup>b</sup> and Alexandros Feresidis<sup>a</sup>**

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<sup>b</sup>*University of Southampton, United Kingdom*

### **Abstract**

Infrared (IR) metasurfaces with sub-wavelength nanoscale features have emerged as a revolutionary tool to manipulate the properties of electromagnetic waves. In particular, the manipulation of the electromagnetic wave in the spectrum from 0.75 to 25  $\mu\text{m}$  could find applications in biomedical, defence and civilian sectors. However, it is challenging to design such types of surfaces since the majority of the materials (thin layers) show uneven optical properties in the IR spectrum. Additionally, the low-cost mass-production of large-scale IR metasurfaces remains a technological challenge. The main attribute of the suggested Al:ZnO (AZO) meta-surface is its ability to modulate the infrared emissivity, or alternatively, the reflectivity of an incident electromagnetic wave in two distinct spectral bands, the 3–5  $\mu\text{m}$  mid-wave and the 8–13  $\mu\text{m}$  long-wave infrared. The proposed metasurface design approach is

based on the operation of metallo-dielectric periodic structures. Furthermore, it exploits the dispersion of material response with wavelength to effectively control electro-optic emissivity with a broadband response within the two distinct spectral bands. In this work, we present a design that makes use of a novel 5-layer stack and includes the AZO periodic array and a thin Ti layer as distinguishing characteristics. The strong material dispersion provided by the low-conductivity AZO array is critical to the design as its periodicity allows the electro-optic emissivity spectrum variation. The thin Ti-film controls the coupling between the top and bottom dielectric spacer, as its strong dispersion properties provide a convenient spectrally selective mechanism. The proposed approach and materials are suitable for CMOS-compatible mass-production manufacturing, bringing IR metasurface coatings closer to commercially relevant and scalable technology.

## Cold Electron Transport in Two-Dimensional van der Waals Nanoelectronics

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<sup>b</sup>*Department of Electrical Engineering, University at Buffalo, The State University of New York, USA*

### Abstract

With the rise of semimetal graphene (Gr) in 2004, two-dimensional (2D) materials including transition metal dichalcogenides (TMDs) and hexagonal boron nitride (h-BN) are considered one of the most promising material candidates for next-generation energy-efficient nanoelectronics owing to their fascinating properties, such as quantum confinement within sub-1-nm thin bodies and atomically sharp van der Waals (vdW) junction interfaces. In this talk I will present our recent study on emerging 2D materials and hetero-structures, especially their novel out-of-plane charge transport and the relevant applications in nanoelectronic devices. We investigated Gr-enabled cold electron injection where the Gr acts as the Dirac source to provide the cold electrons with a localized electron density distribution and a short thermal tail at room temperature. These cold electrons correspond to an electronic refrigeration effect in monolayer MoS<sub>2</sub> and WSe<sub>2</sub>, which enables a transport factor lowering and thus a steep-slope switching mechanism for MoS<sub>2</sub> and WSe<sub>2</sub> field-effect transistors (FETs). Especially, a record high sub-60-mV/decade current density (over 1 μA/μm) can be achieved compared to conventional steep-slope technologies such as tunneling FETs or negative capacitance FETs using 2D or 3D channel materials. Our work demonstrates the potential of a 2D Dirac-source cold electron transistor as a steep-slope transistor concept for future energy-efficient nanoelectronics.

## Effect of Thermal Boundary Resistance on Thermal Management of Interconnects in Logic Chips

Tianzhuo Zhan

*Toyo University, Japan*

### Abstract

The half-pitch size of interconnects in logic chips will scale down below 10 nm in the forthcoming sub-5-nm era, as predicted by the International Roadmap for Devices and Systems (IRDS). The Joule heat produced in the narrowing interconnects can cause a significant temperature rise, which will degrade the performance and reliability of logic chips due to the electromigration effect. Thermal boundary resistance (TBR) between the interconnects and dielectric interlayer dictates the overall thermal resistance of the nanoscale interconnect film stacks, which should be decreased for the thermal management of the interconnects in logic chips. In this study, we investigated the TBR between the interconnects and dielectric interlayer. The measured TBR varies from  $1 \times 10^{-8}$  to  $1 \times 10^{-7}$  m<sup>2</sup> K W<sup>-1</sup> depending on the interlayer used. Simulations by a three-dimensional electrothermal finite element method demonstrate that such a high TBR can cause a temperature increase of hundreds of degrees in advanced logic chips. Hard X-ray photoelectron spectroscopy of deeply buried layers and interfaces reveals that the TBR is dependent on the bonding strength of interfaces adjacent to the interlayer. This study provides a guideline for the thermal management of interconnects in logic chips.

## Ultrafast Terahertz Spectroscopy and Floquet Engineering in a 3D Dirac Semimetal Cd<sub>3</sub>As<sub>2</sub>

Natsuki Kanda<sup>a,b\*</sup>, Yuta Murotani<sup>a</sup> and Ryusuke Matsunaga<sup>a,b</sup>

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<sup>b</sup>PRESTO, Japan Science and Technology Agency, Japan

### Abstract

Optical properties of topological Dirac semimetals are attracting growing interest because 3D massless electrons show unique electromagnetic responses with a large interaction volume with light, providing a fascinating platform for studying ultrafast control of matter and promising application in optoelectronics and nonlinear optics. Their unique infrared responses originate from the gapless band structure, where interband and intraband transitions occur in a near energy scale. To thoroughly derive their novel functionalities, in-depth understanding of nonequilibrium broadband complex response functions is indispensable. We have developed a phase-stable time-domain spectroscopy system in the multiterahertz (10–50 THz) range and studied ultrafast dynamics of a photoexcited Cd<sub>3</sub>As<sub>2</sub> thin film with 30-fs time resolution. We found that photoexcited carriers largely suppress the multi-terahertz refractive index due to the elevated plasma frequency. We also investigated the response function during the formation of Floquet-Bloch state. Under 30-THz narrowband pump, the conductivity spectrum is dominated by stimulated Rayleigh scattering, which resonates between the Floquet subbands and is remarkably enhanced by the elevated plasma frequency.

## Asymmetry at Ferromagnet/Antiferromagnet Interface: Route Toward an Advanced Spin-orbit Torque Device

Chao-Yao Yang

National Yang Ming Chiao Tung University, Taiwan

### Abstract

The antiferromagnet (AFM) and ferromagnet (FM) interface is a unique branch of magnetism of broad scientific interest. AFMs play an important role in spin-orbit torque (SOT) devices based on their ability to generate spin-polarized current and exchange bias when combined with FMs. Since the exchange bias of the AFM/FM bilayer appeared to be tailorable by SOT, it opens a great opportunity for AFM-based spintronics technology that the SOT can modify the spin texture of AFM and FM can serve for detection. In this talk, several AFM/FM systems will be demonstrated for studying the interfacial dynamics of AFM spins. An interesting spin-orbit torque (SOT) ratchet involving the exchange spring effect in an IrMn/CoFeB bilayer device with perpendicular anisotropy and exchange bias is developed. The combined use of electrical and spectroscopic analysis reveals that the exchange spring in IrMn/CoFeB bilayer yields unidirectional anisotropy, resulting in a collinear/orthogonal AFM/FM spin configuration at the interface upon switching CoFeB magnetization upward/downward. The ratcheting characteristics resulting from unidirectional anisotropy manifest in SOT switching. In this process, magnetization against the exchange spring features digital-like switching with a sharp transition, whereas the reverse function is characteristic of analog switching with a gradual transition tail. The dual digital-analog characteristics of the IrMn/CoFeB bilayer may be of benefit in neuromorphic and memory applications.

## Photocontrol of Structural Colors in Self-organized Helical Superstructures

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### Abstract

Light-driven cholesteric liquid crystals (CLCs) exhibit unique selective reflection, originating from their inherent

self-organized helical superstructures, and dynamic reflection tuning in response to light, which has unique advantages for remote, temporal, local, and spatial manipulation. Such elegant systems may represent ideal candidates for use as “photonic inks” to realize changeable information in color reflective displays, especially those providing paper-like viewability in sunlight where backlit devices perform poorly.

In this report, we demonstrate several new strategies for manipulating the structural colors of CLCs. We design a tristable chiral switch by incorporating two different azobenzenes into one chiral structure. Three stable configurations of the chiral switch endow the CLC with two continuous and adjacent tuning periods of the reflection, covering not only entire visible spectrum, but also one more wide period within near-infrared region. The resultant CLCs are capable of creating images of RGB colors with a black background, which is realized based on piecewise reflection tuning. In addition, we proposed a novel tuning mechanism based on a partial photochemical phase transition to enable continuous patterning of photostationary RGB colors in a CLC system, which contains nonresponsive chiral dopants and *o*-fluoroazobenzenes (Fazo) to serve as the photoswitch. Distinct isomer ratios of Fazo result in precise light-directed RGB colors for the photostationary states, and, thus, a fixed relationship is established between the light stimulus and the reflection color. Accordingly, the RGB color patterns can be continuously erased and rewritten under light irradiation with different wavelengths.

## Electrically Switchable Intervalley Excitons with Strong Two-phonon Scattering in Bilayer WSe<sub>2</sub>

Mashaël M. Altaïry<sup>a,b,†</sup>, Erfu Liu<sup>a,†</sup>, Ching-Tarng Liang<sup>c</sup>, Fu-Chen Hsiao<sup>c,d</sup>, Jeremiah van Baren<sup>a</sup>, Takashi Taniguchi<sup>e</sup>, Kenji Watanabe<sup>f</sup>, Nathaniel M. Gabora<sup>g</sup>, Yia-Chung Chang<sup>c</sup> and Chun Hung Lui<sup>a</sup>

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<sup>g</sup>Canadian Institute for Advanced Research, MaRS Centre West Tower, Canada

### Abstract

We report the observation of Q $\Gamma$  intervalley exciton in bilayer WSe<sub>2</sub> devices encapsulated by boron nitride. The Q $\Gamma$  exciton resides at  $\sim 18$  meV below the QK exciton. The Q $\Gamma$  and QK excitons exhibit different Stark shifts under an out-of plane electric field due to their different interlayer dipole moments. By controlling the electric field, we can switch their energy ordering and control which exciton dominates the luminescence of bilayer WSe<sub>2</sub>. Remarkably, both Q $\Gamma$  and QK excitons exhibit unusually strong two-phonon replicas, which are comparable to or even stronger than the one-phonon replicas. By detailed theoretical simulation, we reveal the existence of numerous ( $\geq 14$ ) two-phonon scattering paths involving (nearly) resonant exciton-phonon scattering in bilayer WSe<sub>2</sub>. To our knowledge, such electric-field-switchable intervalley excitons with strong two-phonon replicas have not been found in any other two-dimensional semiconductors. These make bilayer WSe<sub>2</sub> a distinctive valleytronic material with potential novel applications.

## Resistive Switching in Prussian Blue Analog Films

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## Abstract

The physical and chemical properties of Prussian blue analogs (PBA) have increasingly attracted the attention of the scientific community due to its promising applications in electrochemical sensing, electrochromic devices, batteries, supercapacitors, and magnetic/ photomagnetic systems and others. Recently, we have studied the resistive switching effect in electrodeposited Prussian Blue (PB) and Prussian White (PW) films enabling potential applications in the field of electronics. However, electrical property characterization of PBA in combination with control of morphology and structure are rarely investigated. In this work, the relationship between structural properties and resistive switching behavior of electrodeposited PBA films will be discussed (see Figure 1). The structural characterizations were performed with electron microscopy in combination with Raman spectroscopy and different xray techniques.

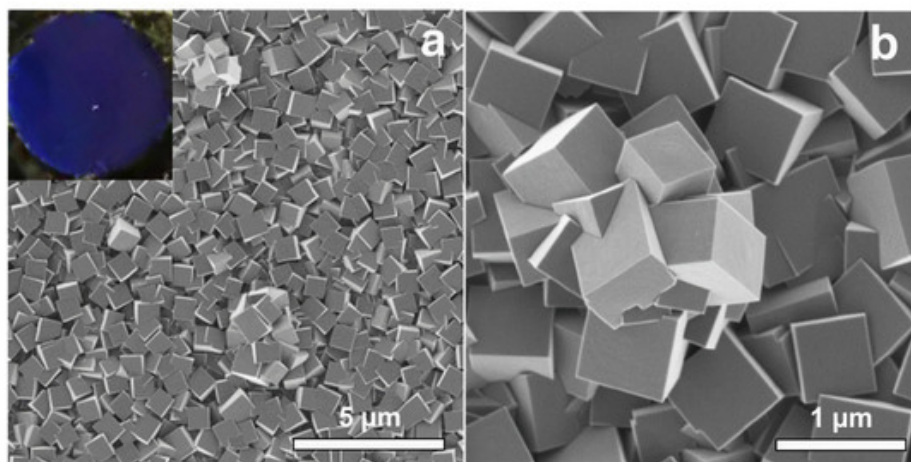


Figure 1. Field emission scanning electron microscope (FEG-SEM) images of electrodeposited Prussian blue (PB) films grown at 0.3 V: (a) surface overview, photograph image of the film (inset), (b) detailed view of the film surface.

## Sustainable Synthesis of Highly Stable Copper Particles with Low-temperature Sintering Capability

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<sup>b</sup>Free University of Brussels, Belgium

<sup>c</sup>Institute of Materials Science of Barcelona, Superior Council of Scientific Investigations, Spain

## Abstract

Copper is an interesting metal, widely used in a myriad of fields including catalysis, additives, electronics, conductive inks and antimicrobial applications. Most of these applications are highly dependent on preserving the metallic nature of copper particles as oxidation alters the chemical, optical and electronic properties of copper limiting its use in these application spaces. Over the years, several methodologies have been adopted to mitigate oxidation of copper such as formation of bimetallic or alloyed particles with more stable metal/transition oxide shells protecting the core copper, fabrication of composites with other conductive material such as graphene and conducting polymers, partially embedding in substrates and use of ligands as capping agents. The use of ligands has proven to be very effective as small molecule ligands can provide sufficient protection to copper without disrupting flow of electrons between adjacent particles and therefore, particularly important for conductive applications. This talk will focus on novel, green approaches to synthesising ligand-capped metallic copper particles under ambient atmospheric conditions. The resulting metallic particles exhibit technologically important properties including, excellent oxidative stability, thermal stability, conductivity, catalytic activity and low temperature sintering capability. The latter is particularly beneficial for flexible electronics, as most of the substrates have low glass transition temperatures making them unsuitable for conventional high temperature processing. The benign nature of all chemicals and solvents used,

together with the low temperature processing conditions, makes these copper particles a suitable material for diverse applications.

### Acknowledgement

We thank the Propulsion Futures Beacon of Excellence at the University of Nottingham for funding.

## Young Researcher Presentations

### Development and Characterization of a Cu<sub>2</sub>O Nanonet as a p-type TCO for Optoelectronics Applications

Mouncif Belmouhoub<sup>a,b</sup>, Gabin Ternin-Rozat<sup>a</sup>, Muriel Braccini<sup>b</sup>, Jean-Luc Deschanvres<sup>a</sup>, Hervé Roussel<sup>a</sup> and Céline Ternon<sup>a</sup>

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#### Abstract

Transparent conductive oxide (TCO) materials are a class of semi-conductor showing two main properties: conductivity, that can be tuned from insulating via semiconducting to conducting, and transparency in the visible range. N-type are well known, in contrary to their P-type counterpart. The design of a performant P-type transparent conductive oxide could lead to the breakthrough of transparent electronics. For that, various compounds have been studied, and especially copper based materials, and for this work, cuprous oxide Cu<sub>2</sub>O. Here, the nanowire (NW) structure was chosen because of its exceptional properties and in particular the opportunity to obtain a single crystalline material. When nanowires are randomly dispersed on a surface to form a percolating network, a new innovative structure called a nanonet is formed. Nanonets have great fault tolerance, high surface area, enhanced electrical and mechanical properties and are easy to integrate in functional devices due to their macroscopic size. Two methods of Cu<sub>2</sub>O NW synthesis have been explored and achieved, the first through direct oxidation of pure Cu NWs under air with the study under controlled atmosphere ongoing. The second by direct hydrothermal synthesis, using low temperature method without any toxic products for humans or the environment. Those two methods will be compared, and the chemical, structural, and electrical properties through the phenomena of percolation of the different nanonets will be displayed in this study.

### Electromagnetic Interference Shielding Performance of Multilayered Metallic Thin Films: Theoretical and Experimental Data

Hyun Jun Kwon\* and Su Jeong Suh

Sungkyunkwan University/Advanced Materials Science and Engineering, Republic of Korea

#### Abstract

The electromagnetic wave shielding efficiency of metallic multilayer thin films was analyzed by comparing the theoretically calculated value with the trend of actual data values. It has been previously demonstrated that the total conductivity of multilayer films was not directly related to the electromagnetic interference shielding efficiency of the films. Therefore, herein, the effect of the electrical conductivity of each layer on the electromagnetic interference shielding efficiency of multilayer films was analyzed in detail. The electrical conductivity was measured by making Cu and NiFe single layer thin films by electroplating. Based on the measured electrical conductivity values, the optimal conditions for multilayer were found by comparing the three-layer(M3) and five-layer structures(M5). The maximum shielding efficiency of M5 was -82 dB. Moreover, the experimental and theoretical shielding efficiencies of M3 presented similar trends in the GHz region. The more stable result of the M3 seems to be a difference due

to the presence of (inter)layer with a critical thickness of less than 200 nm. In order to identify the electromagnetic wave shielding efficiency of the metallic multilayer, a vector network analysis, focused ion beam, scanning electron microscopy, four-point probe, X-ray diffraction, and inductively coupled plasma-optical emission spectroscopy were performed.

## Fabrication of Organic-Inorganic Hybrid Perovskite Single Crystal Lateral Heterojunction and its Application in Optoelectronic Devices

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<sup>a</sup>Information Materials and Intelligent Sensing Laboratory of Anhui Province, Anhui University, People's Republic of China

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<sup>c</sup>Hefei Comprehensive National Science Center, People's Republic of China

### Abstract

Heterojunctions were widely studied as semiconductor structure for photoelectronic devices such as solar cells and photodetectors, due to their ability of dark current reduction and self-powered operation. As a promising material, perovskite have received a wealth of attention from the fields of solar energy, lasers and photodetectors due to its excellent physical characteristics in the past ten years. Although tremendous progress has been made based on perovskite polycrystalline thin films, the inherent abundant surface defects and grain boundaries in polycrystalline thin films will serve as charge carriers capture and recombination centers, unavoidably hindering the charge transfer. Furthermore, the research of perovskite-based heterojunction photodetectors mainly focused on different-halide-ions-based polycrystalline films with vertical structure, which will lead to loss of incident light and interfacial accumulation of defects as well as phase separation. In present work,  $\alpha$ -FAPbI<sub>3</sub>/MAPbI<sub>3</sub> single crystals concentric annular lateral heterojunction was successfully fabricated by liquid phase epitaxy. The  $\alpha$ -FAPbI<sub>3</sub>/MAPbI<sub>3</sub> single crystals lateral heterojunction-based photodetector exhibits high responsivity of 27.50 mA W<sup>-1</sup>, specific detectivity of  $7.71 \times 10^{11}$  Jones, fast response speed of 62.7  $\mu$ s as well as self-powered ability. These results suggest that lateral perovskite single crystal heterojunctions with the same halogen are promising configurations for photodetectors and other optoelectronic devices and systems.

## Air-stable Photodetector with High Specific Detectivity Based on Single-wall Carbon Nanotube/silicon Heterojunctions

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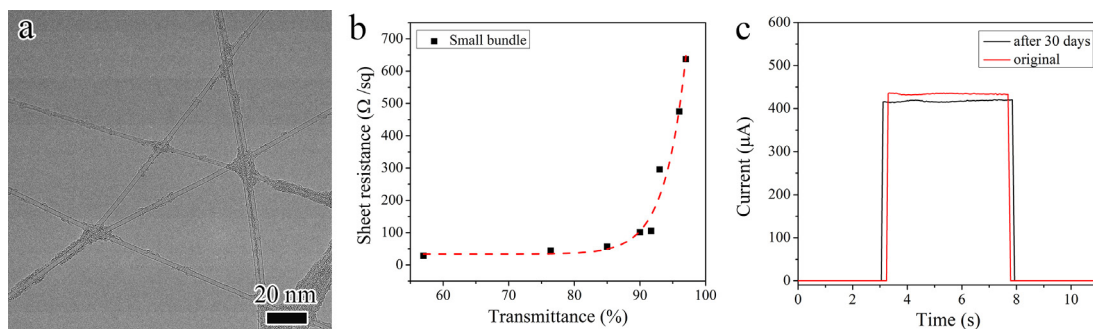
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<sup>d</sup>Shenzhen Geim Graphene Center, Shenzhen International Graduate School, Tsinghua University, PR China

### Abstract

Photodetectors have very important applications in solar cells, aerospace industry, military industry, spectroscopy, a variety of biochemical sensors. Single wall carbon nanotubes (SWCNTs) exhibit excellent optoelectronic properties and have great potential for optoelectronic applications. However, the performance of large-area SWCNT/n-Si heterojunction-based photodetectors has been limited by the quality and photoelectric property of the SWCNT films used. We prepared a carbon-welded, small-bundle SWCNT film (Fig. 1a) with low junction resistance and high transmittance. More than 85% of the bundle size is less than ~10 nm, and the average SWCNT diameter is ~2 nm. The percentage of the junctions with a carbon-welding structure is ~86%. The square resistance of the SWCNT

film reached 100  $\Omega$ /sq at 90% transmittance (Fig. 1b), which is much lower than that of previously reported CNT films for photodetection. SWCNT/n-Si heterojunction-based photodetectors with active areas of 9–900 mm<sup>2</sup> were fabricated. Their best responsivity (R) and detectability reached 0.43 A/W (Fig. 1c) and  $4.2 \times 10^{13}$  Jones, respectively, for a 890 nm laser. The detectors also showed good stability with a 97% R value retained after exposed in air for 30 days, and a broad spectral response (540–2000 nm).



**Figure 1:** (a) Typical TEM image and (b) square resistance with different transmittance of the small-bundle with carbon-welded SWCNT film; (c) the photoresponse of the photodetector with 9 mm<sup>2</sup> window area under 890 nm laser (input laser power=1mW)

## Modification of Optical Parameters of Solid Polymer Electrolyte Films for Optoelectronic Device Applications

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<sup>b</sup>Department of Physics, S.S Arts College and T.P Science Institute, India

### Abstract

It is very important to find the desired optical bandgap materials with suitable bandgap for photonic and optoelectronic device applications. This study reports the optical properties of Hydroxypropyl methylcellulose solid polymer electrolyte films. The solution casting technique was successfully introduced to make salted HPMC films with different salt concentrations. In the spectral range of 200–750 nm, various optical parameters including optical conductivity, optical dielectric function, Urbach energy, etc., were analyzed. Salt showed a significant effect on the optical properties of the host polymer. The absorption edge plays a very important role in energy device applications, here edge was widely displaced towards a region of higher wavelength. The samples showed significant band gap variation and achieved the lowest bandgap for the highest salt doped sample. Also, the optical band gap was effectively employed as a substitute technique for finding the band gap. Tauc's extrapolation method was effectively used to find the type of transition and also the acceptability of Penn's model is also discussed in this paper. In the meantime, XRD results showed a decrease in crystallinity of the host polymer with dopant salt concentration, which directly supports the observed variation of Optical parameters.

## Intrinsic Magnetism in van Der Waals Semiconductors in Their 2D Limit

Ellenor Geraffy<sup>a\*</sup>, Magdalena Birowska<sup>b</sup>, Shahar Zuri<sup>a</sup> and Efrat Lifshitz<sup>a</sup>

<sup>a</sup>Schulich faculty of Chemistry, Solid State Institute, Russell Berrie Nanotechnology Institute and the Quantum information Center, Israel

<sup>b</sup>Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Poland

### Abstract

Ultrathin 2-D van der Waals (vdW) semiconductor materials have procured scientific and technological interest since the discovery of single layered graphene in 2004. Similar to graphene, transition metal trichalcogenides, with the general chemical formula MPX<sub>3</sub> (M= 1st row transition metals, X = chalcogenides), possess fast electron transport

and strong spin orbit coupling without the drawback of no bandgap. These vdW inorganic lamellar compounds are characterized by strong intralayer covalent bonding and weak vdW interaction between adjacent layers. Transition metal atoms endow these materials with magnetic (either ferromagnetic or antiferromagnetic Neel, zigzag or stripy) and magneto-optical properties which can be utilized for new generation 2D magnets and opto-spintronic devices. Yet, the fundamental understanding of these materials as well as the manipulation of their intrinsic magnetism via external stimuli remains to be an unexplored endeavor.

FePS<sub>3</sub> exhibits an overall zigzag antiferromagnetic ordering with previous investigations showing a giant linear dichroism. However, little investigations have been carried out on its intrinsic magnetism and the impact external factors such as temperature and external magnetic field impose on the material.

In this talk, the unique internal magnetic features of bulk FePS<sub>3</sub> using temperature dependent photoluminescence (PL) and magneto-PL measurements are explored. We confirm the presence of a metamagnetic phase transition in FePS<sub>3</sub> upon inducing thermal fluctuations in the material using temperature dependent PL. Additionally, g-factor enhancement in bulk FePS<sub>3</sub> is reported for the first-time using magneto-PL and circular polarized magneto-PL.

## Characterization of Deposited Conductive Ink Layers for Fitness and Use as Rapid Prototyped RF Components

**Christopher Bolton**

*New Jersey Institute of Technology, USA*

### Abstract

With constant advancements in additive CNC-based manufacturing, there is a growing need to determine how accurately a fabricated part will perform compared with theoretical design parameters and Finite Element Method (FEM) modeling. In particular, conductive inks and printed metallic layers are being used for rapid prototyping of a variety of electronics such as component connections, flexible circuit boards, and antenna structures and may be embedded on or within a printed thermoplastic or other dielectric layer. A critical parameter for determining functionality and electrical performance is the uniformity of the metallic layer, as well as how the ink performs in comparison to a bulk material or perfect conductor. A figure of merit for this parameter would be sheet conductance at the intended operational frequency of the printed RF component. Metallic ink samples are fabricated using a variety of deposition techniques including micro-dispense, drop on demand, and reel-to-reel printing methods, as well as by Mayer rod and spin coating procedures. Terahertz Time Domain Spectroscopy and THz imaging are used to characterize inconsistencies in metallic ink layers resulting from manufacturing techniques as well as model the sheet conductance of the ink layer. These nondestructive evaluation techniques are used to expose manufacturing defects and variations in uniformity which could lead to undesirable electronic performance of the printed parts. The application of this analysis will assist in determining viability of additive RF components in critical applications.

## Session: Future Materials for Energy and Sustainability

### Featured Presentations

## Chemical Bonding and Thermoelectric Properties of Materials

**Yuri Grin**

*Max Planck Institute for Chemical Physics of Solids, Germany*

### Abstract

Substantial information sources for the development of materials are the composition-crystal structure-properties relationships. For thermoelectrics, such diagram is multidimensional with complex interplay of its components.

The phenomenon of thermoelectricity is thought to be well understood from the physical point of view, and the main components of thermoelectric behavior – electric and thermal conductivity and Seebeck coefficient can even be calculated with reasonable reliability assuming the knowledge of the crystal structure of the material. Different chemical aspects important for thermoelectric properties like lone pairs, Van-der-Waals bonds, valence band convergence etc. are still under consideration. Chemical bonding, understood as a system of physical forces within a chemical entity, creates a natural bridge between chemical and physical properties of materials. Systematic quantum chemical studies show that atomic interactions play a key role in the chemical and structural organization of thermoelectric materials. On the one hand, bonding forms the basis for the band structure and the total electron balance in the material regulating electron concentration and transport (electron engineering). On the other hand, atomic interactions influence the heat transport in the materials as well (phonon engineering). Spatial distribution of regions with different types of chemical bonding – bonding inhomogeneity and anisotropy - influences especially the thermal transport.

## Photodoped ITO Nanocrystals Unlock Multiple Electron Transfer

Andrea Rubino\*, Michele Ghini, Andrea Camellini and Ilka Kriegel

*Functional Nanosystems, Istituto Italiano di Tecnologia (IIT), Italy*

### Abstract

Transparent conductive oxides nanoparticles are promising materials, with attractive high performances at low cost. One of the best known in optoelectronics are the Indium Tin Oxide (ITO) nanocrystals (NCs). Among their properties, the Localized Surface Plasmon Resonance (LSPR) is crucial, being responsible for the conductive character, thanks to the excess of extrinsic charges resulting from the aliovalent doping of the oxide. More recently, the photodoping, a light-driven charge accumulation of electrons induced by multiple absorption events of high-energy photons emerged as a contactless and promising tool to promote a further increase in charge density through a zero environmental impact post-synthetic treatment. Photodoping of ITO NCs results in the reversible accumulation of tens to hundreds of electrons per single NC. Due to the proportionality between the plasmonic peak energy ( $\omega_{\text{LSPR}}$ ) and the free carrier density, the storage and depletion of photodoped electrons can also be analysed by monitoring the spectral evolution of the LSPR. The light-driven charge accumulation can give access to processes involving multiple charge transfers, being also beneficial in terms of efficiency. Here, we report a first evidence, in the case of photo-doped ITO NCs, of the multiple-charge transfer process, counting in more than one electron, by means of a gradual oxidative treatment using an electron-acceptor molecule, the F<sub>4</sub>TCNQ. This phenomenon encourages even more the use of these semiconductors in the field of solar energy conversion, but also in related fields such as photoelectrochemistry and photocatalysis.

## Influence of Silicon on the Calendering Behavior and Properties of Anodes for Lithium-Ion Batteries

Sören Scheffler<sup>a,b\*</sup>, René Jagau<sup>a,b</sup> and Arno Kwade<sup>a,b</sup>

<sup>a</sup>*Institute for Particle Technology/Technical University of Braunschweig, Germany*

<sup>b</sup>*Battery LabFactory Braunschweig/Technical University of Braunschweig, Germany*

### Abstract

The growing electrical mobility market requires improvement in the energy density of batteries as a key factor for reaching higher driving range. Thus, enhanced specific gravimetric and volumetric capacity of lithium-ion batteries (LIB) is required. There are different ways to enhance the energy density, for example, by the usage of new active materials or calendering of the electrodes.

As a future active material, silicon has a specific capacity that is ten times higher compared to commonly used graphite (3579 compared to 370 mAh/g). However, the usage of silicon comes along with a significant drawback: during lithiation and de-lithiation a large volume change of silicon takes place (approx. 280%). The aim of this

study is to identify the influence of varied silicon contents on the electrode behavior during calendaring and their mechanical properties and electrochemical performance. The mechanical properties of the anodes are quantified by adhesion strength as well as elastic and plastic deformation behavior.

The produced anodes are calendared to create a variation in the coating density and mechanical properties. During calendaring, with the usage of higher silicon contents a higher line load is required to achieve comparable coating densities resulting in an increased compaction resistance of 229.7 N/mm (10 wt% Si) compared to 131.7 N/mm (pure graphite). After calendaring, a decrease of the adhesion strength from 1.42 MPa to 0.97 MPa of the electrode coating is detected which can be explained by damage to the binder network and an increased springback of the silicon-rich electrodes.

## Electrochemical Nitrogen Reduction Reaction for Renewable Ammonia Generation

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### Abstract

As a vital feedstock to pharmaceutical, manufacture fertilizers, and other chemical products, ammonia ( $\text{NH}_3$ ) is also regarded as a promising energy carrier with low liquefying pressure and high hydrogen density, which lead to a significant fixation reaction from the inexhaustible nitrogen ( $\text{N}_2$ ) into  $\text{NH}_3$ . Due to the thermodynamic stability of the  $\text{N}_2$  molecule, the  $\text{N}_2$  fixation is still severely confined. The Haber–Bosch process is a century-old method and regarded as the most important industry for  $\text{NH}_3$  manufacture, while it requires abundant iron-based catalysts and harsh operating conditions (400–600 °C and 150–350 atm). As a result, the Haber–Bosch process would cause 1.4% of the world's energy consumption and 1.6% of total global  $\text{CO}_2$  emission, resulting in the exploration of sustainable  $\text{N}_2$  fixation systems under ambient conditions an important issue. Electrochemical  $\text{N}_2$  reduction reaction (NRR) is an emerging technology to reduce  $\text{N}_2$  into  $\text{NH}_3$  under ambient conditions that is powered by renewable energy. Recently, one of the main research points locates on the exploration of advanced electrocatalysts to activate the inert  $\text{N}_2$  molecule and alleviate the energy barriers for  $\text{N}_2$  reduction. In our work, we have developed several potential electrocatalysts and put forward several technique strategies for  $\text{N}_2$  reduction to overcome the existing two main challenges in the NRR: (1) the binding force between electrocatalyst and  $\text{N}_2$  is too weak due to the poorly optimized structure of the electrocatalyst; (2) the adverse hydrogen evolution reaction is regarded as an intense-competing reaction towards NRR that should be suppressed.

## Enhanced Light-to-hydrogen Conversion Using Plasmon Core-shell Photocatalysts

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### Abstract

Hydrogen ( $\text{H}_2$ ) is being extensively studied as an ideal energy era for transportation, energy storage, and electricity generation. Hydrogen fuel provides high energy efficiency and zero-carbon byproducts, which addresses issues pertaining to sustainability, environmental emissions, and energy security future. As a potential approach, light-driven water splitting, which dissociates water molecules into hydrogen and oxygen, is significantly useful for artificial photosynthesis. Thus, light-driven hydrogen and oxygen production reactions can be employed in green energy communities with low-carbon emission due to the inexhaustibility, universality, and environmentally friendly processes. Plasmon core-shell photocatalysts (e.g.,  $\text{Au@CeO}_2$ ,  $\text{Au@CeO}_2/\text{Graphene}$ ) are recently emerging as the promising candidates for light-to-fuels conversion purpose. Such entities, on the one hand, provide unique physical properties such as large surface areas and high activities and stabilities in relation to its counterparts. On the other, their optoelectronics properties are greatly improved accordingly. That is, the hot electron-hole pairs are produced and transferred into the plasmonic Au and doped  $\text{CeO}_2$ -related materials under the irradiation of the

light, meanwhile the Graphene shell can serve as a conducting candidate to extend the lifetime of the plasmon-excited hot charge carriers migrating from the activating cores in nanocomposite systems. As a result, plasmonic core-shell photocatalyst designs can significantly limit the recombination rate of generated hot pairs to promote the photocatalytic redox reactions and apparent quantum yield efficiency. The present studies can bring a bright perspective for light-to-fuel conversions, in particularly for green and renewable hydrogen fuels production.

## Perspectives on Improving the Safety and Sustainability of High Voltage Lithium-Ion Batteries Through the Electrolyte and Separator Region

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### Abstract

Lithium-ion batteries (LIBs) are promising candidates within the context of the development of novel battery concepts with high energy densities. Batteries with high operating potentials or high voltage (HV) LIBs (>4.2 V vs Li<sup>+</sup>/Li) can provide high energy densities and are therefore attractive in high-performance LIBs. However, a variety of challenges (including solid electrolyte interface (SEI), lithium plating, etc.) and related safety issues (such as gas formation or thermal runaway effects) must be solved for the practical, widespread application of HV-LIBs. Most of these challenges arise in the region between the electrodes: the electrolyte region. This review provides an overview of recent development and progress on the electrolyte region, including liquid electrolytes, ionic liquids, gel polymer electrolytes, separators, and solid electrolytes for HV-LIBs applications. A focus on improving the safety of these systems, with some perspectives on their relative cost and environmental impact, is given. Overall, the new information is encouraging for the development of HV-LIBs, and this review serves as a guide for potential strategies to improve their safety, allowing the development of HV-LIBs, including solid-state batteries, to be accelerated to practical relevance.

## Poly(ionic liquid)-in-salt Electrolytes for Next Generation of Batteries

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### Abstract

Cationic poly(ionic liquid)-in-salt (PolyIL-IS) is emerging as a new promising polymer electrolyte (PE) for the development of future solid-state batteries that can utilize different metal ion resources, including lithium, sodium and potassium. Similar to the polymer-in-salt system proposed by Prof Angell nearly three decades ago, the PolyIL-IS can achieve higher ionic conductivities at elevated salt concentrations. Meanwhile, a relative high metal ion transference number (> 0.5) has been also obtained in both Li and Na electrolytes. This is expected to address the challenges associated with PE, that is achieving high metal ion conduction and transference numbers simultaneously, which is crucial for its practical applications. Based on computational studies, we gain an in-depth understanding of the role of salts in this material, elucidating the metal ion transport mechanism and the chemical environment for fast metal ion transport. A computational electrolyte design strategy is also presented to assist the efficient design of PolyIL-IS electrolytes. The experimental validations yield promising results in the Na system, obtaining a good conductivity of around 1 mS/cm at 80 °C and stable cycling against Na metal anode up to 100 hours in a symmetric cell. Our work opens up a new avenue for designing future polymer electrolytes.

## Enhancing Comprehensive Energy Storage Properties of Tungsten Bronze $\text{Sr}_{0.53}\text{Ba}_{0.47}\text{Nb}_2\text{O}_6$ -Based Lead-free Ceramics by B-Site Doping and Relaxor Tuning

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### Abstract

Dielectric ceramics with relaxor characteristics have the potential to meet the demand for capacitors of next generation pulse devices. In this work, a lead-free Sb-modified ( $\text{Sr}_{0.515}\text{Ba}_{0.47}\text{Gd}_{0.01}$ ) ( $\text{Nb}_{1.9-x}\text{Ta}_{0.1}\text{Sb}_x$ ) $\text{O}_6$  (SBGNT-based) tungsten bronze ceramic is designed and fabricated for high-density energy storage capacitors. By using a B-site engineering strategy and incorporating Sb into the B-site of the SBGNT-based tungsten bronze ceramic, it is possible to improve the relaxor characteristics of the ceramic through the structural distortion of the polar unit BO<sub>6</sub> and the modulation of polarization. More importantly, the inhibition of abnormal growth of non-equiaxed grains can benefit SBGNT-based ceramics by suppressing the conductivity and leakage current density, thereby enhancing the breakdown strength. This is supported by the electrical impedance spectra. Consequently, a remarkable, comprehensive performance is realized via balancing recoverable energy density ( $\sim 3.26 \text{ J/cm}^3$ ) and efficiency (91.95%) simultaneously at 380 kV/cm, which surpasses the pristine sample without the Sb dopant (2.75 J/cm<sup>3</sup> and 80.5%, respectively). The corresponding ceramics display superior stability in terms of fatigue ( $10^5$  cycles), frequency (1~200 Hz), and temperature (20~140 °C). Further charge-discharge analysis indicates that a high-power density (89.57 MW/cm<sup>3</sup>) and an impressive current density (1194.27 A/cm<sup>2</sup>) at 150 kV/cm are achieved simultaneously in the tungsten bronze relaxors, making them promising lead-free candidates for dielectric energy storage applications.

## Direct Room Temperature Synthesis of $\alpha$ -CsPbI<sub>3</sub> Perovskite Nanocubes – Implications for Photovoltaic and Electronics Applications

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### Abstract

Cesium lead iodide perovskite nanocrystal (CsPbI<sub>3</sub> PNCs) is a promising material for efficient solar cells and red light-emitting diodes, especially for the cubic-structured  $\alpha$  polymorph with its ideal bandgap energy. However, it had only been accessible via the hot-injection synthetic method, which requires precise temperature control and hence have limited scalability and industrialization potential. This challenge is unique to cesium lead iodide perovskite nanocrystals and is the only composition still inaccessible to room temperature among all ABX<sub>3</sub>-type perovskite nanocrystals. Here, we report the first room temperature, one-pot synthesis of  $\alpha$ -CsPbI<sub>3</sub> PNCs in open air, achieved by optimized ligand-solvent combinations to control crystallization kinetics and phase preference of CsPbI<sub>3</sub>. The resulting 6.0 nm sized,  $\alpha$ -phased nanocubes have photoluminescence peaks at 642 nm (full-width half-maximum:

44 nm) and absolute quantum yields up to 83% after purification. The method is simple, reproducible, scalable, and generalizable to other cesium lead halide and formamidinium lead iodide PNCs.

## BlueP/Janus MoSSe van der Waals Heterostructure as an Efficient Anode Material for Lithium-Ion Batteries

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### Abstract

Developing high-capacity anode materials for Lithium-Ion Batteries (LIBs) with high energy density, abundant resources, environmental benignity, and low cost is an essential strategy to tackle non-renewable energy sources. We explored the importance of BlueP-Janus MoSSe heterostructure for LIBs anode using Density Functional Theory (DFT) calculations. The thermal stability of the above material is characterized by ab-initio molecular dynamics (AIMD) simulations, whereas phonon spectral studies confirm the dynamical stability of the material. Besides, the in-plane Young's modulus and Poisson's ratio indicate outstanding mechanical strength. The BlueP-Janus MoSSe heterostructure has a strong adsorption affinity towards Li at various surfaces and interfaces. More importantly, Li can diffuse both at the inside and outside surface of the heterostructure with short diffusion distances. The small open circuit voltage (OCV) signifies their extraordinary properties to be suitable for increasing the working potential of electrode materials for Li-ion batteries. The negligible lattice change during lithiation implies that the 2D BlueP-Janus MoSSe heterostructure can withstand massive volume change with good cyclic performance. The above findings may provide valuable insights for improving the performance of rechargeable LIBs.

## High-capacity Mixed Cu-Fe Sulfides: Towards Sustainable Batteries with Prussian Blue Derivatives

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### Abstract

The steep rise of battery demand requires the development of battery materials that are more sustainable and easier to recycle, substituting costly and strategic elements like Li, Ni, and Co with widely and more evenly available ones like Na and Fe in the electrode materials. Prussian blue (PB) and its analogues (PBA, AM[M'(CN)<sub>6</sub>]) are cheap, non-toxic, water and air-stable, and can be entirely synthesized by water-based methods, therefore being highly sustainable. Given PBA porous framework, they have been used as templates to prepare the so-called PB derivatives (PBD), which present many compositions, including metal oxides, sulfides, carbides, hybrids, and an array of morphologies. In this work, the PBA copper iron hexacyanoferrate(II) (CuPB) is explored as a precursor to producing mixed Cu/Fe sulfides for Lithium-ion batteries. Dopamine or tannic acid is added to the system and polymerized in situ to control the particle size during CuPB growth. The presence of the polymers favors K-rich CuPB, while the thickness of the polymer shows a key role in preventing particle coarsening during the sulfidation process and enables its application in LIB, which otherwise is prohibited due to lack of structural and electrochemical stability. Through mild thermal treatment conditions (300 °C, 10 min), carbon-coated (K)CuFeS<sub>2</sub> is produced. Standard coating with n-methyl-2-pyrrolidone and polyvinylidene fluoride binder is explored in addition to greener alternatives like ethanol and polyvinylpyrrolidone to process the PBD for electrochemical testing. The carbon-coated KCuFeS<sub>2</sub> electrodes provided a reversible capacity of up to 800 mAh/g at 10 mA/g with nearly 100% recovery after rate handling. After 500 cycles at 250 mA/g, the electrodes still provided a capacity of 380 mAh/g.

## Octahedral Cluster Compounds: A New Promising Member of the Restricted Family of Ambipolar Materials for Sun Light Energy Conversion

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### Abstract

Ambipolar materials are a class of compounds that can intrinsically transport and transfer simultaneously both charge carriers, holes and electrons in a comparable way. Unlike conventional unipolar semiconductors in which a type of charge carrier is predominant, ambipolar materials can display p-type and n-type characteristics within a single device, which makes them attractive materials for many different application fields such as sunlight conversion. Only few materials such as semiconducting polymers, carbon nanotubes, 2D materials or organic-inorganic hybrid perovskites exhibit ambipolar behaviors. Their intriguing intrinsic electronic properties result from their specific electronic structures widely tuned by their morphology, composition and size.

The authors recently investigated the ambipolar character of Mo<sub>6</sub> clusters compounds. Transition metal cluster (MC)-based halides and chalcogenides are nano-objects that have a tri-dimensional size restriction giving them fascinating optical and electronic properties such as molecule-like energy gaps, strong absorption in the visible and/or NIR spectral regions, deep red luminescence or high (photo)catalytic effectiveness. Outstanding ambipolar properties of MC compounds were highlighted through a range of photoelectrochemical characterizations and led to the design, as a demonstrator, of an all solid solar cell integrating an MC-based light-harvester. Thus, this presentation will be firstly focused on the evidence of the ambipolar character of Mo<sub>6</sub> cluster iodides, from its origin to its interest for solar energy conversion, before to generalize these new outstanding properties to the octahedral cluster family through the investigation of Re<sub>6</sub> and mixed (Re,Mo)<sub>6</sub> sulfides and selenides.

## Towards Controllable Liquid Foams for Photocatalytic Applications

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### Abstract

Soap films have extraordinary properties with a remarkable potential to inspire unconventional design in a variety of technological applications. Although the first interest in some of these properties dates back to some centuries ago, the complex physical-chemical phenomena underlying these peculiar emerging characteristics has for long time remained poorly explored. In recent years, the advent of nanotechnologies and the continuous effort in the research of the optimal design in miniaturized engineering systems, has driven interest of the scientific community towards a deeper understanding of these fascinating objects. In the framework of the SOFIA project (Soap Film based Artificial Photosynthesis, H<sub>2</sub>O<sub>2</sub>-FETOPEN-2018-2019-2020- 01), soap films are being investigated towards their exploitation as soft, adaptive membranes for solar fuel production. The ambitious goal of the project is indeed to investigate and realize an innovative photosynthetic system, capable to produce fuel out of the reduction of carbon dioxide via the complex photochemical processes that can be triggered in soap films, when exposed to sunlight, in controlled and properly defined conditions. Among the different ongoing activities within the project, in this talk we particularly present those related to soap film and soap foam characterization and modeling, targeted to obtain specific foam structures to be exploited for photocatalytic applications.

## Recycling Real-World Waste Plastics via Thermal Catalytic and Plasma Processes for Co-Production of Hydrogen and High Value-Added Carbon Products

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### Abstract

The growing demand for plastic products in our daily lives generates massive amounts of waste each year. Further enhanced by the COVID-19 pandemic, the use of single-use medical plastic materials (such as masks and gloves) for health protection has resulted in a significant increase in (micro)plastic post-consumer waste. The current disposal routes are mainly thermal utilization (incineration) and landfill, which is energy intensive and environmentally unfriendly. More efficient and sustainable recycling methods are desperately needed to turn the waste plastics into value-added chemicals or materials. Non-thermal plasma (NTP) technologies have received intense attention and are very attractive to convert the waste plastics in a fast and efficient way. NTPs generate high-energetic electrons and highly reactive species, opening up new reaction pathways and allowing thermodynamically unfavorable reforming reactions to happen at a low energy input. Here, we report a breakthrough concept combining an atmospheric pressure microwave plasma with tailor-made perovskite-type catalysts for the co-production of hydrogen and value-added carbon composite products. The effect of different process parameters and catalyst types on the gas production and carbon species was systematically studied for thermal catalytic and plasma processes. The produced value-added carbon products using different perovskite-type catalysts were characterized by various state-of-the-art techniques with respect to the quantity and quality of carbon materials establishing the correlation with reaction temperature and catalyst type. We provide a new efficient and sustainable route for waste plastic management together with a fast frontier for co-production of hydrogen and high value-added carbon materials.

## Graphene Oxide from Graphite of Spent Batteries as Support of Nanocatalysts for Fuel Hydrogen Production

Renata Pereira Lopes<sup>a</sup>, Gabriel Henrique Sperandio<sup>a</sup>, Iterlandes Machado Junior<sup>a</sup> and Esteffany Lima Bernardo<sup>a</sup>

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### Abstract

The demand for energy storage devices has been increase over the last years, increasing the amount of waste generated at the end of its lifespan. Among these residues, Zn-C batteries stand out, which have a cathode made of graphite carbon, which can be used as a precursor for graphene oxide (GO). This work aimed to synthesize GO from spent Zn-C batteries to support metallic nanoparticles (Co and Ni) for use in borohydride catalysis to produce hydrogen gas. Hydrogen is considered the fuel of the future. However, it presents problems of storage and transport. NaBH<sub>4</sub> is considered a hydrogen storage, being solid at room temperature and easily transported. One mole of borohydride generates four moles of hydrogen. Although thermodynamically feasible, the reaction is kinetically slow. Therefore, the development of nanocatalysts is very important. These ones, however, agglomerate easily. The support allows to disperse the nanoparticles, avoiding their agglomeration, obtaining greater efficiency. In addition, the catalyst can be reused in various catalytic cycles. In this work, GO was synthesized according to the adapted Hummers method. The obtention of GO was confirmed by X-ray Diffraction and Raman Spectroscopy techniques. Ni and Co nanoparticles were deposited to GO in the ratio (60:40 w/w) showing excellent results of hydrogen evolution from borohydride catalysis. The material was reused over three cycles, showing the same efficiency. It can be concluded that it was possible to obtain a new material with added value from Zn-C batteries, with potential use in the evolution of hydrogen from borohydride catalysis.

## Metal Chalcogenide Thin Films by Chemical Methods for Photoelectrochemical Applications

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### Abstract

Chalcogenide semiconducting thin films have gained attraction as semiconductor materials in applications such as photovoltaics, photoelectrochemical cells and optoelectronic devices. These materials are earth abundant and nontoxic with good optical absorption ( $\alpha \geq 10^5 \text{ cm}^{-1}$ ) in the visible and near infrared region of the solar spectrum. In this contribution the development of ternary chalcogenide semiconductor materials such as  $\text{CuSbS}_2$ ,  $\text{Sb}_2(\text{SSe})_3$  by electrodeposition technique will be outlined. Electrodeposition is a scalable and low-cost technique which can be carried out at room temperature nucleation and growth mechanisms along with the optimization of the bath conditions and its effects on the optoelectronic properties are discussed. The phase purity, structure, and optoelectronic characteristics of the material were studied extensively using experimental tools such as XRD, XPS, SEM, photosensitivity, etc. The photoelectrochemical performance of  $\text{CuSbS}_2/\text{CdS}/\text{Pt}$  and  $\text{Sb}_2\text{Se}_3/\text{CdS}/\text{Pt}$  will be compared.

## Young Researcher Presentations

### Effect of $\text{Al}_2\text{O}_3$ , SiC and TiC Nanoparticles on the Properties and Microstructure of Direct Chill Cast Al MMnCs

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### Abstract

The addition of hard ceramic reinforcement nanoparticles to aluminium for producing aluminium metal matrix nanocomposites (Al MMnC) can be an effective method to increase the strength of aluminium alloys. The aim of this research is to produce Al MMnCs through direct chill (DC) casting in order to improve properties after downstream processing. In this study, 6xxx series aluminium alloys reinforced by different particles including alumina ( $\text{Al}_2\text{O}_3$ ), titanium carbide (TiC) and silicon carbide (SiC), exhibiting sizes ranging from the nano to sub-micro-scale, were investigated. Lab scale composite DC cast billets with a diameter of 80 mm were produced by ultrasound-assisted stir casting technology, in attempts to overcome the main challenge of particles agglomerating. Mechanical testing and microstructural analysis were subsequently performed to understand the effect of different particles and processing parameters on the resultant microstructure and mechanical properties. Whilst the addition of  $\text{Al}_2\text{O}_3$  nano-reinforcement did not result in any significant changes to the mechanical properties, a ~9% and ~18% increase in the yield strength (YS) of the alloy was achieved through the addition of 1 wt% TiC reinforcement or 1 wt% SiC reinforcement, respectively, with the latter also producing an increase of ~7% in the ultimate tensile strength (UTS). These results are discussed and analysed further in this study, with plans for implementation in pilot line production assessed.

### Selective Borohydride Oxidation Reaction on Ni Catalyst at the Anode of Direct Borohydride Fuel cells

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## Abstract

Direct borohydride fuel cells (DBFCs) are operated to liquid reactants at the anode and cathode for generating electricity. It could be utilized as a power source without air supply in the space and under the water. The reactants for the DBFC are sodium borohydride ( $\text{NaBH}_4$ ) stabilized with sodium hydroxide ( $\text{NaOH}$ ) solution and hydrogen peroxide ( $\text{H}_2\text{O}_2$ ) stabilized with sulfuric acid ( $\text{H}_2\text{SO}_4$ ) solution at the anode and cathode, respectively. Platinum-group metals (e.g. Pt and Pd) are currently used as the catalyst on both electrode sides in DBFCs. Palladium catalysts are a well-known catalyst for BOR at the anode of DBFCs. However, their high cost and low abundance limit the practical applicability in DBFCs. On the other hand, nickel is comparably more abundant and considered an alternative anode catalyst in DBFC research. A facile, direct nickel catalyst synthesis method using nickel precursor and cation or anion exchange ionomer (CEI or AEI) mixture on nickel foam are developed for anode electrode in DBFC. The selective catalytic activities for the borohydride oxidation reaction and hydrogen oxidation reaction are the key parameters for achieving high-performance DBFC. The local pH atmosphere (high local pH at the AEI layer, and low local pH at the CEI layer) is one of the parameters for the selective BOR at the anode. The nickel catalyst naturally has high selective BOR due to the high over potentially deposited hydrogen binding energy ( $\approx 0.9$  eV) than palladium catalyst ( $\approx 0$  eV). The practical applications of DBFC are becoming more realistic thanks to the utilization of non-noble Ni catalysts.

## Hollow Urchin-like Nickel Cobaltite as Oxygen Evolution Reaction Catalyst for Anion Exchange Membrane Water Electrolyzers

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## Abstract

Hierarchical hollow urchin-like nickel cobaltite was synthesized using a two-step hydrothermal method. The effects of metal composition and surfactant addition on the morphology, structure, and electrochemical performance towards oxygen evolution reaction (OER) in alkaline medium were investigated. Addition of cetyltrimethylammonium bromide (CTAB) reduced the aggregation of particles, which translated to a high electrochemically active surface area and electrical conductivity. Decreasing the Ni content from 1.0 to 0.25 did not alter the morphology and structure of the product to any extent. Nonetheless, among the materials of different Ni and Co compositions,  $\text{NiCo}_2\text{O}_4$  exhibited the most excellent OER electrocatalytic performance, achieving an overpotential of 380 mV, which is comparable to those of the benchmark OER catalysts. It also performed good in an anion exchange membrane water electrolyzer (AEMWE) using 1 M NaOH at 60 °C, reaching a current density of about 420 mA/cm<sup>2</sup> at a cell voltage of 1.95 V. Lowering the electrolyte concentration and operating temperature led to a decline in electrocatalytic activity. In general, this study is essential for the realization of affordable electrolyzer technology based on transition metal catalysts.

## Waste Tire-derived Carbon Obtained from Green Hydrothermal Route as Anode Material for Alkali-ions Batteries

Loris Berardo\*, Abdelfattah Mahmoud, Audrey Schrijnemakers, Frédéric Boschini and Rudi Cloots

Greenmat, University of Liege, Belgium

## Abstract

For a few years, the use of hydrochar as anode materials in alkali-ions batteries has been investigated. Hydrochar is a carbon powder made by hydrothermal carbonization (HTC) of wet biomass and biodegradable wastes. However, biomass and biodegradable wastes are not the only sources of carbon and other wastes should be considered, such as

plastics or rubbers. Among them, scrap tires are currently a major environmental concern and thus, an ideal candidate for a waste valorization project. However, despite organic wastes, scrap tires contain a significant number of heavy metals or undesired elements, such as nano-SiO<sub>2</sub>, Fe, Zn, Pb, Co, or Al. These elements could interfere during the cycling of the carbon material and drastically hamper the electrochemical performances. Currently, research focuses on harsh treatments, such as concentrated sulfuric acid and hydrofluoric acid, to remove heavy metals. However, such treatments can become hazardous during upscaling and leads to economic and environmental issues. Therefore, the focus of the present work is to develop an appropriate method to i) degrade and purify scrap tires by a green hydrothermal process to remove unwanted heavy metals and obtain a leached carbon and ii) process the leached carbon into an electrochemically active carbon used as an anode material in alkali-ions batteries (Li, Na, and K-ion).

## Boosted Zn<sup>2+</sup> Storage Performance of Hydrated Vanadium Oxide by Defect and Heterostructure

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### Abstract

Aqueous Zn-ion battery (ZIB) is regarded as a promising alternative to the lithium-ion battery due to its attractive advantages such as the large volumetric capacity (5,851 mAh mL<sup>-1</sup>), abundance, safety, and inexpensiveness. However, the high polarization and large atomic mass of the bivalent Zn<sup>2+</sup> cause sluggish insertion kinetics, low Coulombic efficiency, and unsatisfactory rate performance. In this study, we demonstrated that a heterostructure in the form of defective hydrated vanadium oxide embedded in the porous carbon textile (d-VOH@CT) could tackle these issues. The additional edges created by crystal defects significantly promoted facile zinc-ion adsorption and intercalation. Expanded interlayer spacing and reduced crystalline domain size kinetically facilitated fast zinc-ion diffusion in d-VOH flakes with shortened diffusion paths. Moreover, the heterostructure of d-VOH on the conductive carbon textile triggered rapid charge transfer, leading to high rate capability and structural stability. The ZIBs fabricated using the d-VOH@CT cathode delivered a preferable reversible capacity of 416 mAh g<sup>-1</sup> at 0.1 A g<sup>-1</sup>, an impressive energy density of 293 Wh kg<sup>-1</sup> as well as long cycle life. In addition, the d-VOH@CT heterostructure was able to be used as a freestanding cathode for a flexible ZIB with outstanding mechanical robustness and electrochemical stability.

## Enhanced Electrochemical Performance of V<sub>2</sub>O<sub>5</sub> Prepared by Spray Drying Process as Cathode Material for Zinc-ion Batteries

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### Abstract

The search for alternatives to lithium-ion battery (LIB) is mainly driven through some inherent disadvantages like cost or safety and through a predicted energy supply problem that is just around the corner. The rechargeable aqueous zinc-ion battery (ZIB) is seen as a sustainable, safe, low cost and ecological alternative to LIBs. The cathode is currently the limitation component of this energy storage technology, using metallic zinc as anode material and aqueous electrolytes. For instance, only a few cathode materials have been investigated as suitable hosts for Zn<sup>2+</sup>: manganese-based, vanadium-based, prussian blue analogs, and more recently organic materials.

Our research focus on vanadium pentoxide V<sub>2</sub>O<sub>5</sub> because it can deliver a high theoretical capacity of 589 mAh.g<sup>-1</sup> based on the two-electron redox centers. Nevertheless, vanadium-based materials are affected by poor electrical

conductivity and volume changes caused by  $Zn^{2+}$  insertion/extraction during cycling. Several strategies can be used to improve electrochemical performance: insertion of metal ions or structural water in cathode material, optimization of architecture design and selection of conductive additives. The main objective of this study was to tailor the morphological design through a one-step spray-drying process at pilot scale. The results demonstrate the strong influence of this process on morphological and electrochemical properties. Spray-dried  $V_2O_5$  exhibit remarkably high capacities of  $495 \text{ mAh.g}^{-1}$  and  $240 \text{ mAh.g}^{-1}$  at low ( $0.1 \text{ A.g}^{-1}$ ) and high current density ( $5 \text{ A.g}^{-1}$ ) respectively, excellent rate capability and good stability. Therefore, the  $V_2O_5$  prepared by spray drying offers good qualities to be used as cathode material in ZIBs.

## Cobalt Molybdenum Sulfide as Alternative Cathode for Anion Exchange Membrane Water Electrolyzers

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### Abstract

Green hydrogen is an important energy carrier for energy transition and water electrolysis is considered the most promising process for its large-scale production. Through this process, water is reduced at the cathode to produce high-purity hydrogen. The anion exchange membrane water electrolyzer (AEMWE) configuration has the potential to operate at high current densities, besides to allow the use of PGM-free catalysts; both very relevant features. Hence, our goal is to propose earth-abundant cathodes for AEMWE.

Transition metal sulfides were hydrothermally synthesized and physicochemically characterized, which enabled a better comprehension of their electrocatalysts' behaviour. In an AEMWE cell, a current density of  $1.2 \text{ A cm}^{-2}$  was obtained at 2 V for cobalt molybdenum sulfide ( $\text{Co}_{0.5}\text{Mo}_{0.5}\text{S}_x$ ) cathode. In addition,  $\text{Co}_{0.5}\text{Mo}_{0.5}\text{S}_x$  presented good stability in 40 h of operation, besides most of its current density decay proved to be recoverable. Finally, post-mortem  $\text{Co}_{0.5}\text{Mo}_{0.5}\text{S}_x$  gas diffusion electrode was analyzed by FEG-SEM, including EDS technique, and Raman spectroscopy.

## The Role of Interface of $\text{CuO}_x$ - $\text{TiO}_2$ Hybrid Metal Oxide in Enhancement of Oxygen Reduction Reaction Performance

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### Abstract

Energy security and clean energy are of increasing importance given the current scenario. Hence fuel cells and metal-air batteries are gaining significant attention in recent times. However, the major problem associated with these technologies is the sluggish nature of oxygen reduction reaction (ORR) and the expense associated with the catalyst. This study reports nitrogen-doped carbon-supported  $\text{CuO}_x/\text{TiO}_2$ -based heterostructure ( $\text{CuO}_x/\text{TiO}_2$ -10 wt%/NC-800) as an efficient, durable, and low-cost ORR catalyst.  $\text{CuO}_x/\text{TiO}_2$ -10 wt%/NC-800 catalyst is synthesized using a simple hydrothermal method. The catalyst has excellent ORR activity with onset potential and half-wave potential of 0.90 V and 0.80 V vs. RHE, respectively. It also shows outstanding limiting current density of  $5.80 \text{ mA cm}^{-2}$ . The catalyst offers excellent stability (with 92% current retention after 24 h) and durability (only 25 mV half-wave potential shift after 2000 CV cycles). The catalyst follows the  $4e^-$  transfer process ( $n = 3.94$ ) with rather nominal amount of hydrogen peroxide formation (3.5%). The enhanced ORR activity is attributed to the strong synergistic effect between  $\text{CuO}_x/\text{TiO}_2$  and NC. The unique structure formation also helps to get excellent electronic conductivity, large surface area, appropriate porosity, and desirable interface charge transfer between  $\text{CuO}_x$  and  $\text{TiO}_2$ .

## Novel Photoswitchable and Hydrophobic Thermoplastic Polyurethane for Potential Energy Applications

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### Abstract

Renewable energy utilization *via* a smart material has recently gained much interest in the development of sustainable modern technologies. Among smart materials, photoswitchable materials are attractive in the utilization of solar energy. Herein, a novel type of azobenzene based thermoplastic polyurethane (Az-PU) was synthesized using a diisocyanate as the hard segment, a polymer diol as the soft segment and an azobenzene diol as the chain extender for the photoisomerization effect, through step growth polymerization with four different ratios of the building blocks. The structure of Az-PU was characterized by Fourier transform infrared spectroscopy and nuclear magnetic resonance. The resulting optimal polymer with a 3:2:1 ratio for diisocyanate:polymer diol:azobenzene diol possesses a weight average molecular weight of 183,900 g/mol, and a water contact angle of  $106.3 \pm 4.1^\circ$ , along with tensile strength  $6.9 \pm 0.71$  MPa, Young's modulus of  $50.1 \pm 5.3$  MPa, elongation at break of  $78.6 \pm 0.2\%$ , and energy at break of  $3.6 \pm 0.4$  J/m<sup>3</sup>. The polymer shows a heat release enthalpy of 64.8 J/mol after UV irradiation (325 nm) for 5 minutes at 100 W. During UV irradiation, the photon energy is stored in the isomers of the molecule, which can be retrieved in the form of heat by a triggered release or a self-decay process. This smart recyclable polymer could be a promising sustainable material for developing efficient solar energy harvesting, storage and utilization.

## High Concentration Electrolytes for Wider Operational Voltage Aqueous Rechargeable Na-ion/S Battery

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### Abstract

The aqueous rechargeable sodium-ion batteries are attracting great attention compared to their organic counterparts in terms of safety, ionic conductivity and cost-effectiveness but suffer the limited energy density and low output voltage due to narrow electrochemical stability window of water and the unavailability of high-capacity electrode material. In that context, multiple electron transfer and earth abundant sulfur considered as a future electrode material due to high theoretical capacity ( $1675 \text{ mAh g}^{-1}$ ) and energy density. However, the polysulfide shuttling and the formation of unrecoverable H<sub>2</sub>S gas significantly hamper their performance. Since, the polysulfide dissolution is an interfacial phenomenon and depend upon both the electrolyte and electrode material. Therefore, it is important to tune both the components for achieving high performance. Compared to dilute electrolytes, in highly concentrated "water-in-salt" (WiSE) or "water-in-bi-salt" electrolytes (WiBS), most of the water molecules involve in solvation shells and are unavailable as free molecules, which reduces water activity significantly and increase stability window upto ~3 V. Thus, coupling the WiSE or WiBS with appropriate sulfur host can enhance the battery performance by reducing the water activity and preventing the polysulfide dissolution.

Herein, we target the development of a sodium-ion/S battery with a WiSE or WiBS and conductive sulfur host as an electrode material exhibiting high specific capacity. Further, the polysulfide dissolution at different salt concentrations, cycles, operating times and depth-of-discharge was investigated by various electrochemical, chemical and visualization studies. In future, we plan to move towards commercialization of our battery.

## The Surface Charge Neutralized TENG Output Depending on Humidity Condition

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## Abstract

Triboelectric nanogenerator (TENG) produces electric energy from static electricity. The static charges come from the contact between two materials, such as metal and dielectrics. Electric charges move on a metal electrode under the influence of electrostatic induction. In this work, we show that electric fields from charged dielectrics cause polarization of metal electrodes and generate a net charge through the charge neutralization process. The output voltage depends on the initial charge balancing of I-V measurements, even with the same moving charge density. It can be explained as two kinds of charges; one is fixed, and another is movable. The kinds of electric charges in the TENG cause the output voltage difference. The movable charges affect current and voltage output. Conversely, fixed charges affect open-circuit voltage. The fixed charge retention can be affected by the environment of water vapor in the air. The humidity-dependent output characteristics explain the electrical binding and fixed charge movement in our system TENG.

## Mxene@nitrogen-doped Carbon Films for Supercapacitor and Piezoresistive Sensing Applications

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## Abstract

A simple strategy is proposed to fabricate MXene@nitrogen-doped carbon (MC) composite film by vacuum filtration followed by annealing. PDA nanospheres serve as spacers, carbon precursor, and nitrogen sources, and meanwhile endow MC with porous networks. Nitrogen doping improves the electrochemical performance of MC, while the porous network increases the ion transport rate and the sensitivity to strain. When assembled into a symmetrical supercapacitor, the device delivers a high energy density of 23.2  $\mu\text{Wh}\cdot\text{cm}^{-2}$  at a power density of 317.7  $\mu\text{W}\cdot\text{cm}^{-2}$ . The assembled all-solid-state zinc-ion hybrid supercapacitor delivers a much higher energy density of 61.24  $\mu\text{Wh}\cdot\text{cm}^{-2}$  at a power density of 352.76  $\mu\text{W}\cdot\text{cm}^{-2}$ . The MC-based wearable sensor exhibits a sensitivity of 0.21  $\text{kPa}^{-1}$  at a pressure range of 0–2 kPa for piezoresistive sensing with a superior durability over 2000 cycles. This multifunctional MC composite film has promising potentials for the fabrication of energy storage devices and wearable electronics.

## Study of Piezoelectric Behavior of Semiconducting Nanonets

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## Abstract

An innovative and promising alternative for future electronics is the integration of semiconducting metal oxide Nanonets in devices, which are two dimensional network of interconnected nanowires randomly oriented in the plane. The merits being easy low cost integration process with high fault tolerance, good reproducibility and large surface area with little knowledge available regarding the piezoelectric behaviour of these random horizontally oriented nanowires. Studies will thus be conducted on determining the piezoelectric behaviour of Nanonets incorporated on flexible substrate. Upon successful integration of nanonets on kapton based substrate, mechanical stress will be applied to nanonets under given electric bias in the form of bending and traction to study their Electro-Mechanical behaviour. Bending tests will be conducted to understand the current evolution in nanonet with changes in radius of curvature of flexible substrate. In parallel, Traction test will help us in getting information regarding the current evolution characteristics on exposure to elongation and compression in nanonet structure. Conducting these measurements under SEM will give information about changes in nanonet structure at time zero. Finally, combining

these SEM observation with electrical measurements under traction for various device geometries will give us better understanding of piezoelectric behaviour of our nanonet.

## **Electrospun $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>/PAN Nanofibers Mat: A Multifunctional and Efficient Platform in Wastewater Treatment**

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### **Abstract**

The previous decade has seen incredible progress in the identification of important materials and their vastly diverse characteristics at the nanoscale. Nanoscale particles have provided scientists with a new tool for understanding and exploiting natural phenomena that occur when metals and particles are structured at the nanoscale. It is feasible to expand the capabilities of electrical equipment while also reducing their size, power consumption, and weight with the use of nanotechnology. Water purification technologies on the cutting edge are the entry point for wastewater treatment. Heavy metals, chemical dyes, and pharmaceutical medication contamination in water bodies have a negative impact on human health when consumed. As a result, there is an urgent need to create an effective and self-powered membrane-based platform that aids in the removal of heavy metals, organic dyes, and pharmaceuticals from wastewater treatment management. In this paper, I introduce a revolutionary Electrospun nanofibers mat that can successfully decolorize the solution after filtering even at greater concentrations. In addition to investigating the multimodality of nanofibers mat, the current study expanded the use of nanofibers mat in heavy metal adsorption. We also accomplished electrochemical drug detection in wastewater treatment. This opens the door to the development of low-cost, highly sensitive, and efficient membranes for wastewater treatment and remediation.

## **Piezocatalytic MB Dye Degradation Using Bi<sub>2</sub>VO<sub>5.5</sub>**

**Manish Kumar\*** and **Rahul Vaish**

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### **Abstract**

Dye effluents are mainly discharged through textile firms which are not self-degradable and needs special treatment. Piezocatalysis and photocatalysis are the new emerging wastewater treatment methods. Bi<sub>2</sub>VO<sub>5.5</sub> powder is a member of the Bi-V-O system which is known to possess ferroelectric property below 725 K. The piezocatalytic property of Bi<sub>2</sub>VO<sub>5.5</sub> has not been explored till now. In this work we synthesized single-phase Bi<sub>2</sub>VO<sub>5.5</sub> powder through solid-state method at 750 °C in 8 hrs. X-ray diffraction and Raman spectroscopy confirmed single orthorhombic phase formation. SEM images acclaimed the formation of the irregular shaped morphology. XPS analysis provided the various elemental oxidation state of the Bi<sub>2</sub>VO<sub>5.5</sub>. Time dependent photocurrent responses were done to understand charge carrier transport in the effect of dark and visible light. The piezocatalysis study affirmed the degradation of methylene blue dye using Bi<sub>2</sub>VO<sub>5.5</sub> with an efficiency of 58% in 240 minutes. To affirm the major radical taking part in the study scavenger test was conducted.

## **Micro-plasma Reactors for Next-generation Manufacturing**

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### **Abstract**

As the world moves toward the electrification of the transportation sector, more efficient means of producing batteries

will be required. Currently, cathode synthesis for commercial lithium-ion batteries requires 90% of the total energy used during cell manufacturing. Cathode synthesis is currently a slow batch process that spans 48–60 hours and batch sizes are limited to control temperatures (up to 1400°C in kilns) across large volumes. We have achieved the world's first atmospheric micro-plasma synthesis of two common commercial cathode materials, nickel manganese cobalt oxide (NMC) and lithium iron phosphate (LFP). Synthesis times using this method have been decreased to approximately 10 seconds from the traditional 48–60 hours span. This short duration also decreases lithium loss which typically occurs during the traditional method. The result is spherical cathode particles approximately 500–900nm in diameter. This novel synthesis method has great promise to revolutionize the battery manufacturing industry and will find an interested audience.

## Influence of Transition Metals Dopants on the Photovoltaic Properties of BaSnO<sub>3</sub>: A First-principles Calculations

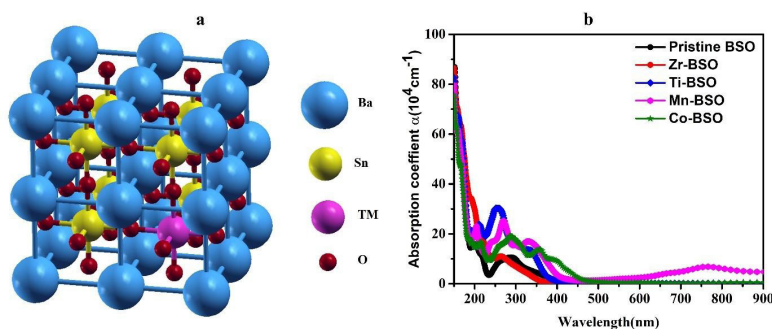
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<sup>b</sup>Laboratory of Condensed Matter and Interdisciplinary Sciences (LaMCS-I), Faculty of Sciences, Mohammed V University, Morocco

### Abstract

BaSnO<sub>3</sub> (BSO) is a popular choice among researchers due to its high transparency for inverted solar cell structure<sup>1</sup>. Transition metal doping is known to influence the optical properties of BSO to a great extent. Accordingly, BaSn<sub>0.875</sub>TM<sub>0.125</sub>O<sub>3</sub> (BSTMO, TM= Zr, Ti, Mn, and Co) compounds were investigated in the framework of first-principles calculations using the full potential linearized augmented plane wave (FP-LAPW) method based on the density functional theory implanted in the wein2k code. The formation energies, optimized lattice parameters, density of states, electron density mapping, electronic band structures, and optical band properties were calculated. It is predicted that the Zr and Ti doped systems could improve the optical transparency of BaSnO<sub>3</sub>, which can be highly suitable for transparent conducting oxides. Besides, the Mn and Co doped systems revealed enhanced optical absorption in the UV-visible region of the solar spectrum, which could be a promising candidate for absorber layers in the photovoltaic cells. The current work establishes a conceptual underpinning for the doping effect in order to enhance the optical properties of BSO, which will aid future experimental research.



**Figure 1:** a) Crystal structure of 2×2× 2 supercell and b) absorption coefficient spectra of BSO and BaSn<sub>0.875</sub>TM<sub>0.125</sub>O<sub>3</sub> (TM= Zr, Ti, Mn, and Co).

## KTiPO<sub>4</sub>F: The Negative Electrode Material for Potassium Batteries

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## Abstract

Lithium-ion batteries (LIBs) play a pivotal role in achieving the key objective “zero-carbon emission” as countries agreed to reach a 1.5°C global warming target according to the Paris agreement. Nowadays, due to the tremendous mobile and stationary consumption of small/large-format LIBs, the demand and consequently the price for such energy storage devices have been raised. The aforementioned challenges originate from the shrinkage of the major applied critical materials in these batteries such as cobalt (Co), nickel (Ni), Lithium (Li), graphite (G), and manganese (Mn). Therefore, it is imperative to consider alternative elements to address issues corresponding to the limitation of resources in the globe. Potassium (K) is considered as an effective alternative to Li since K is a more abundant element, has a higher operating potential, a faster diffusion rate, and the lowest Stokes radius in comparison to the closest neighbors in the periodic table (Li and Na). Among all reported materials for metal-ion batteries, some of them, possessing the general formula  $AMXO_4L$  [ $A = Li, Na, K; M = Fe, Ti, V; X = P, S, Si; L = O, F, OH$ ] is of potential to be applied both as anode and cathode and enable researchers to investigate them in the full symmetric battery format.  $KTiPO_4F$  (KTP structural material) has been previously reported by our group as a promising cathode with decent electronic properties.

Herein, we report a synthesis, crystal structure characterization, morphology, as well as K-ion storage properties of  $KTiPO_4F$ . Our investigation reveals that  $KTiPO_4F$  delivers discharge capacity  $> 150$  mAh/g at 26.6 mA/g (C/5 current rate) in the potential window of 0.001–3 V. Surprisingly, the cycling performance of C- $KTiPO_4F$ //K cell is stable for 1000 cycles at 130 mA/g (C current rate), presenting capacity  $> 130$  mAh/g.

## Clean Water Generation by Utilizing the Photothermal Conversion Properties of Magnetite and Carbon Black Found in E-waste

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### Abstract

Scarcity of clean water has become one of the most recalled issues of the world. Interfacial solar steam generation (ISSG) technique could be a solution to this problem; especially in the third world countries, where electricity is not abundant. Instead of heating bulk water from the bottom of the reservoir, ISSG technique utilizes a solar evaporator to concentrate heat at the site of evaporation, which increases the evaporation efficiency. However, the cost of such evaporators become high due to the fabrication process and cost of the photothermal materials. To fabricate a very cost-effective, scalable, and efficient solar evaporator, waste black photocopier toner is coated on the top surface of used paper-based egg tray. The waste black toner contains Magnetite ( $Fe_3O_4$ ) and Carbon Black, that have photothermal conversion capability. A polyurethane foam is used to make the evaporator float and transport water to the top surface of the evaporator through its interconnected microchannels. The porous and fibrous structure of the egg tray absorbs water quickly due to its hydrophilic nature while the carbon black and magnetite absorb solar energy and convert it to heat that produces steam with 78.5% efficiency at  $1.3 \text{ kg m}^{-2}\text{h}^{-1}$  evaporation rate. Due to the presence of carbon black and magnetite the proposed evaporator demonstrates optical absorption of 96.3% in the UV-Vis-NIR (200 nm–2000 nm) region of solar spectrum. The evaporator shows promising performance in desalination and wastewater purification application by evaporating seawater and model wastewater with 66.16% and 75.33% efficiency, respectively.

## Hierarchical Urchin-like $Cu_xCo_{3-x}O_4$ Spinels as Oxygen Evolution Reaction Catalysts in Alkaline Anion Exchange Membrane Water Electrolysers

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## Abstract

In this work, powdered, hierarchical  $\text{Cu}_x\text{Co}_{3-x}\text{O}_4$  catalysts were used as catalysts for oxygen evolution reaction (OER) in an alkaline anion exchange membrane water electrolyser. The effect of increasing copper concentration on the morphology, structure, and OER catalysis performance of Cu-doped spinel  $\text{Co}_3\text{O}_4$  was studied. The synthesized  $\text{Cu}_x\text{Co}_{3-x}\text{O}_4$  catalysts had a micro-urchin morphology. With increasing copper concentration, the nanowires forming the urchin-like structures became thinner and finer. The crystallite sizes of the catalysts decreased with increasing Cu-content. These findings support the BET measurements, which demonstrated that the surface area of the spinel catalyst increased with increasing amount of the dopant. In general, Cu-doped  $\text{Co}_3\text{O}_4$  samples performed better than the undoped spinel catalyst possibly due to the higher specific surface area of the Cu-doped catalysts, which provided more active sites for OER. The sample synthesized with Cu-doping at  $x = 0.75$  (CCO-0.75) performed the best among the catalysts tested. At  $10 \text{ mA cm}^{-2}$ , the recorded overpotential in 1 M KOH was 385 mV, which is approximately 24% lower than that recorded for the undoped  $\text{Co}_3\text{O}_4$  sample. CCO-0.75 exhibited good stability even after subjecting it to 2000 cycles of polarization from 0.2 to 0.55 V (*vs. Ag/AgCl*). An alkaline anion exchange membrane water electrolyser was assembled using CCO-0.75 on Ti GDL, Pt/C on carbon GDL, and LDPE-VBC-TMA as the anode, cathode, and anion exchange membrane, respectively. The CCO-0.75||Pt/C only required 1.74 and 1.65 V cell voltage to reach  $100 \text{ mA cm}^{-2}$  at 20, and 60 °C in 1 M KOH solution.

## High-Voltage Stabilization of O3-Type Layered Oxide for Sodium-Ion Batteries by Simultaneous Tin Dual Modification

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## Abstract

O3-type layered oxide materials are considered to be a highly suitable cathode for sodium-ion batteries (NIBs) due to their appreciable specific capacity and energy density. However, rapid capacity fading caused by serious structural changes and interfacial degradation hampers their use. A novel Sn-modified O3-type layered  $\text{NaNi}_{1/3}\text{Fe}_{1/3}\text{Mn}_{1/3}\text{O}_2$  cathode is presented, with improved high-voltage stability through simultaneous bulk Sn doping and surface coating in a scalable one-step process. The bulk substitution of  $\text{Sn}^{4+}$  stabilizes the crystal structure by alleviating the irreversible phase transition and lattice structure degradation and increases the observed average voltage. In the meantime, the nanolayer Sn/Na/O composite on the surface effectively inhibits surface parasitic reactions and improves the interfacial stability during cycling. A series of Sn-modified materials are reported. An 8%-Sn-modified  $\text{NaNi}_{1/3}\text{Fe}_{1/3}\text{Mn}_{1/3}\text{O}_2$  cathode exhibits a doubling in capacity retention increase after 150 cycles in the wide voltage range of 2.0–4.1 V *vs* Na/Na<sup>+</sup> compared to none, and 81% capacity retention is observed after 200 cycles in a full cell *vs* hard carbon. This work offers a facile process to simultaneously stabilize the bulk structure and interface for the O3-type layered cathodes for sodium-ion batteries and raises the possibility of similar effective strategies to be employed for other energy storage materials.

## Development of Flexible, Self-powered Gas Sensor Based on Poly(vinylidene fluoride)/MoS<sub>2</sub>-BaTiO<sub>3</sub> Nanocomposites

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### Abstract

Future generation wearable applications require smart sensing devices with excellent durability and self-powered features. The detection of gas in numerous industries has been widely concerned. However, conventional gas sensors require an external connected power supply, which does not fulfill the low power and self-powered requirements of today's internet of things, limiting its use as a portable device. As a result, an effective and easy self-powered gas sensor for detecting gas at room temperature is required. In this work, we have investigated the Poly(vinylidene fluoride)/MoS<sub>2</sub>-BaTiO<sub>3</sub> composites for the fabrication of self-powered CO<sub>2</sub> gas sensors applications. The nanocomposite MoS<sub>2</sub>-BaTiO<sub>3</sub> have been synthesized by hydrothermal method. The spin coating technique has been used to deposit the composite film on the ITO glass electrode. The structural, thermal stability and surface morphology of the Poly(vinylidene fluoride)/MoS<sub>2</sub>-BaTiO<sub>3</sub> composites film were investigated by X-ray diffraction analysis (XRD), Thermal gravimetric analysis (TGA) and Atomic force microscopy (AFM). The XRD patterns indicate that pure PVDF and its nanocomposites have been successfully synthesized. It's been observed that Poly(vinylidene fluoride)/MoS<sub>2</sub>-BaTiO<sub>3</sub> composites has higher thermal stability as compared to the pure PVDF. The morphology of the film indicates that, with the addition of BaTiO<sub>3</sub>, MoS<sub>2</sub> and BaTiO<sub>3</sub>-MoS<sub>2</sub> composite, the average roughness values are increased (6.227 nm, 4.300 nm and 6.555 nm). Poly(vinylidene fluoride)/MoS<sub>2</sub>-BaTiO<sub>3</sub> composite based gas sensors show high thermal stability, fast response time and high sensitivity as compared to the pure PVDF.

## Coal Polymer Composites Prepared by Fused Deposition Modeling (FDM) 3D Printing

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### Abstract

Coal is a vital energy resource worldwide, but pollutants and greenhouse gases from its combustion cause environmental problems. To explore the non-combustion approach to use and valorize coal, anthracite and lignite

were blended with polyamide 12 (PA 12) through FDM printing and compared in the composites. By adding lignite, Young's modulus improved with increasing loading while tensile strength increased at 20 wt% (44.6 MPa) and slightly decreased at 50 wt% (40.4 MPa), compared to that of PA 12 (42.6 MPa). By contrast, the addition of anthracite decreased the tensile performance at all loadings. Rheology tests and morphology analyses suggested that the interactions between fillers (anthracite and lignite) and PA 12 may cause differences in tensile properties. In addition, the printed lignite composites showed improved thermal conductivity (~2-fold), indicating lignite demonstrates the potential to build functional composites. This work provides a strategy to use lignite in composites by 3D printing for value-added products and reduces the demand for petroleum-based polymers. Our approach diverts lignite from combustion processes and alleviates the negative impact of lignite use on the environment.

## Session: Bio and Soft Materials: Biomedical, Medicine and Other Applications

### Featured Presentations

#### The Impact of Cooperative Motion in Disordered Systems: Primary Relaxation in (extremely) Viscous “Liquids” and Thermal Treatments in Implanted Semiconductors

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#### Abstract

When an energy barrier  $\Delta E$  needs to be crossed in order that a rearrangement of atoms, molecules or monomers occurs in a disordered system, a suitable number  $\Lambda$  of units must necessarily concur to the motion; this is known as “cooperativity”. Such a kind of collective dynamics characterizes, for instance, liquids approaching their glass transition, and is sensitive to the presence of constraints. A suitable thermodynamic potential is introduced [Pieruccini & Tombari; Phys. Rev. E 97, 032116 (2018)], whereby the cooperativity  $\Lambda(\Delta E)$  follows as a consequence of the conservation of the mean chemical potential during configurational fluctuations in systems which, during their evolution, probe a sequence of local phase space potential wells. Applications to the analysis of primary relaxation in polymers (observed through NMR motional narrowing, mechanical, dielectric or calorimetric responses) are briefly illustrated. The main lines of thought underlying the recent application of cooperativity concepts to post-implantation annealing in semiconductors [Boldrini et al.; Mat. Sci. Semicond. Proc. 148, 106825 (2022)] are also presented. Al implanted 4H-SiC systems have been considered in particular, and the effects of annealing temperature and time on the final substitutional fraction  $\phi(T, \text{time})$  are discussed. It is pointed out that the conditions at which implantation itself was previously carried out (e.g. temperature and dose rate) affect significantly the effectiveness of post-implantation treatments. Some preliminary idea about the possibility to describe these effects in terms of cooperative motion is briefly outlined.

#### The Influence of Process Parameters on the Selected Properties of Ti6Al7Nb Alloy Surface Structured in Fluorine-based Plasma

Anna Jedrzejczak<sup>a\*</sup>, Kinga Adach<sup>b</sup>, Mateusz Fijalkowski<sup>b</sup> and Natalia Plusa<sup>a</sup>

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#### Abstract

Titanium alloys are becoming one of the most promising engineering materials in many industries including

medicine, aerospace and automotive sectors. They are characterized by many beneficial properties, among others: excellent mechanical features, biocompatibility and high corrosion resistance. Therefore they are considered one of the most suitable materials especially in medical applications (implants and surgical tools). As the topography and chemical composition of the biomaterials surface are the properties that strongly affect the interaction with cells, the possibility of shaping them can significantly increase their attractiveness and make them better suited for specific applications. Plasma techniques seem to be a very promising tool for this purpose.

In fluorine-based plasma etching processes, various physical and chemical mechanisms affect the profile of the etched surface. Depending on the chemical composition of gases and applied process parameters there is a possibility to modify the morphology of titanium alloy surface adequately to the required applications.

The influence of process parameters applied during the etching (bias and pressure values, chemical composition of plasma and substrate temperature) on selected properties of titanium alloy (Ti6Al7Nb) surface will be presented.

Sulfur hexafluoride (SF<sub>6</sub>) was utilized as a main etching gas and masks with a specific geometry made of stainless steel were used during the process to obtain a pattern on the etched surface.

#### **Acknowledgments:**

This research was financially supported by the Polish National Science Center, research grant no. 2018/31/D/ST5/03581, Project Title: "The investigation of the mechanisms of dry etching of Ti6Al7Nb titanium alloy in fluorine based plasma".

## **A Simulation Study of Microbial Invasion in Fibrous Structures of Avian Eggshell Membrane**

**Seungwoo Sim<sup>a\*</sup>, Sang-Hee Lee<sup>b</sup>, Cheol-Min Park<sup>b</sup>, Sang-im Lee<sup>c</sup>, Haeun Cho<sup>d</sup> and Youngho Cho<sup>a</sup>**

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#### **Abstract**

Avian eggshells can protect themselves from infection despite of continuous exposure to the environment with a great quantity of harmful microorganisms. To understand their antibacterial mechanism, therefore, can provide insight into the development of bio-inspired antibacterial materials. Many of previous studies focused on the chemical defense of eggshells based on antibacterial proteins while physical defense through eggshell microstructures also play an important role for the antibacterial behavior. In the present study we attempted to investigate how effectively the eggshell membranes with fibrous network structure can prevent the microbial invasion through simulation experiments. To do so, we first developed a mathematical model to emulate the migration of microbial particles in the fibrous structure of eggshell membranes, based on the experimental values of microbial size, the number and inter-layer distance of the membrane layers, and etc. Subsequently, we predicted the penetration ratio of the microbial particles through eggshell membranes for the several avian species. We briefly discuss how the results of the present work can be used as the basis for the development of green antimicrobial materials.

## **Silica Nanoparticles as Drug and siRNA Delivery System**

**Gozde Ultav<sup>a\*</sup>, Hayrettin Tonbul<sup>b</sup> and Emine Salva<sup>a</sup>**

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## Abstract

Silica nanoparticles (SNPs) can be produced in small diameters with good reproducibility, stability, and biocompatibility for carrying and delivering drugs or oligonucleotides to reduce the side effects and offers better treatment. Our work, suggests drug and gene encapsulated SNP formulation for ovarian cancer therapy. In this study, we developed a drug-loaded biodegradable SNP formulation with siRNA to ensure tumor suppression. This formulation is also glutathione (GSH) triggered due to the S-S bonds in silica nanoparticle structure. After obtaining the drug-loaded PEGylated and actively targeted silica nanoparticles about 50 nm in size, the characterization studies were performed by SEM and TEM to observe particle size and morphology, zeta potential to observe the positive charge (about +40 mV) on SNP surface (which is important for enabling interaction with negatively charged siRNA). Chemical conjugations were confirmed by FTIR and in vitro drug loading was determined as about 5%. Drug release studies suggest that the SNPs were degraded at GSH introduced media leads to a higher drug release and observed drug release was about 50% at GSH free media after 28 days. Complexations were demonstrated by gel electrophoresis and biocompatibility was determined by in vitro cell culture (L929 cell line) where no cytotoxicity was observed. Determination of cytotoxicity was performed by the HeLa cell line. According to the results, SNPs can deliver both drug and siRNA at the same time which is promising for developing more effective cancer therapy.

## Bioengineering Breast Tumors with Decellularized Porcine Mammary Glands Bioinks

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## Abstract

Breast cancer is the most common cancer in women worldwide. Breast tumors are formed by cancer cells (BCCs), stromal cells, extracellular matrix (ECM) and soluble factors, being all involved in tumor progression. Bioprinted 3D *in vitro* models have emerged as promising platforms to recapitulate tumor architecture and understand cancer physiopathology. The ECM importance in tumor progression has motivated the synthesis of biomimetic bioinks. Among them, decellularized tissues-derived matrices (TDMs) can provide the native biological cues, but its inadequate mechanical properties prevent their bioprinting. The aim of this work is to develop a breast TDM-derived bioink suitable for bioprinting breast cancer models. A method to efficiently decellularize porcine mammary glands and enable its jellification was developed. TDMs were rich in collagen and glycosaminoglycans, but they could not be bioprinted, and it was necessary to add rheological modifiers (TGA). Bioinks were further tuned by adding collagen I (Col1), overexpressed in breast tumors. Hydrogels had Young modulus of  $\approx 4$  kPa, recapitulating tumors stiffness. BCCs had a good viability, forming spheroids with low ecadherin expression. The presence of Col1 into the bioink (TGAC) improved ink printability and shape fidelity, and increased BCCs proliferation but reduced their malignancy and drug resistance. Indeed, TGA showed a fibronectin and multidrug resistance protein 1 upregulation and higher drug resistance provoked by an upregulation of HSP90AB1, suggesting a higher malignancy of BCCs in the absence of Col1. In conclusion, TDM bioinks closely recreate tumor ECM and allow the bioprinting of cancer models with a close recapitulation of BCCs malignancy.

## Young Researcher Presentations

### Magnetic Nanoparticles in Bone Tissue Engineering

Akshith Dasari<sup>a,b\*</sup>, Jingyi Xue<sup>a</sup> and Sanjukta Deb<sup>a</sup>

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## Abstract

Large bone defects with limited intrinsic regenerative potential represent a major surgical challenge and are associated with a high socio-economic burden and severe reduction in the quality of life. Tissue engineering approaches offer the possibility to induce new functional bone regeneration, with the biomimetic scaffold serving as a bridge to create a microenvironment that enables a regenerative niche at the site of damage. Magnetic nanoparticles have emerged as a potential tool in bone tissue engineering that leverages the inherent magnetism of magnetic nano particles in cellular microenvironments providing direction in enhancing the osteoinductive, osteoconductive and angiogenic properties in the design of scaffolds. There are conflicting opinions and reports on the role of MNPs on these scaffolds, such as the true role of magnetism, the application of external magnetic fields in combination with MNPs, remote delivery of biomechanical stimuli in-vivo and magnetically controlled cell retention or bioactive agent delivery in promoting osteogenesis and angiogenesis. In this presentation, I will focus on the role of magnetic nanoparticles for bone-tissue-engineering applications in both disease modelling and treatment of injuries and disease. Furthermore, I will highlight the materials-design pathway from implementation strategy through the selection of materials and fabrication methods to evaluation. Finally, recent advances, unmet needs, current challenges and emerging strategies in bone tissue regeneration will be discussed.

## Development of Curcumin-loaded Niosomes as a Drug Delivery System

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## Abstract

Drug Delivery Systems (DDS) have seen significant progress in the last decade, with a particular focus on nanomaterials. Nanotechnology, by itself, is a fast-growing research area that can overcome limitations associated with drug delivery. One of the crucial challenges of pharmacology is improving efficacy and reducing the side effects of drugs or developing a controlled drug delivery. Nanoparticles play an essential role in overcoming drug delivery limitations since they can protect and carry pharmaceutical materials to the targeted cells. In this research, an optimum formulation of niosome to deliver curcumin to cancerous cells will be introduced; according to a three-level Box-Behnken design and based on dimension and stability, an optimum formulation for bare niosome was prepared. Then curcumin was loaded on the optimum formulation to achieve curcumin-loaded niosomes. Dynamic light scattering, Fourier transforms infrared spectroscopy, and scanning electron microscopy characterized niosomes. Besides stability against temperature changes (range of 5-40 °C), prepared particles were durable at 4 °C for two months. 99.8% drug entrapment efficiency and 68.33% loading capacity were observed for curcumin-loaded niosomes. Prepared systems showed a sustained-release behavior of up to 25.49 ±0.70 % of curcumin during 336 h. The talk will conclude with the cytotoxicity studies. Blank niosome showed no significant toxicity effect on cells at high concentrations, confirming cytocompatibility of the particles. Curcumin-loaded niosomes had dose-dependent toxicity against cancerous cells. The concentration of 200 µg/ml of the drug-loaded carrier, containing 66.75 µg curcumin, showed an IC50 effect after 48 h of explosion with cells.

## Using Polystyrene Beads as Sacrificial Template to Produce Porous Mannitol Particles by a Spray-drying Process for Pharmaceutical Applications

Morgane Valentin<sup>a\*</sup>, Damien Coibion<sup>a</sup>, Crédic Malherbe<sup>b</sup>, Rudi Cloots<sup>a</sup> and Frédéric Boschini<sup>a</sup>

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<sup>b</sup>Mass Spectrometry Laboratory, MolSys Research Unit, University of Liege, Belgium

## Abstract

Nowadays, powder engineering is increasingly considered in the pharmaceutical field to improve the efficiency of drugs by enhancing their physicochemical, micromeritic, physio-mechanical and/or pharmacokinetic properties. Among the different strategies, porous particles are studied to control drug delivery, improve bioavailability and enable tableting. Due to a low hygroscopicity, a stable crystalline structure and a high compatibility with most APIs, mannitol has been chosen as the primary component in this study.

In this work, we present a straightforward approach to produce porous mannitol particles using a spray-drying process with polystyrene beads acting as sacrificial templating agent. Porous particles of mannitol were recovered by chemical etching, replacing toxic solvents (i.e. chloroform and toluene) by ethyl acetate. Scanning electron microscopy allowed us to highlight the formation of hybrid particles after the spray-drying process. The effectiveness of chemical etching has been verified by infrared spectroscopy and thermal analysis. The influence of PS beads on mannitol polymorphism was demonstrated by X-ray diffraction. By modulating the mannitol:polystyrene (M:PS) ratio, microstructure and structural properties of mannitol particles were controlled. The optimal conditions were obtained with a weight ratio of M:PS=1:1, these particles having an average diameter of 2.5  $\mu\text{m}$  and more than 90% of  $\alpha$ -mannitol. Finally, the possibility to produce these porous particles at the pilot scale was investigated.

## Electrospun Polycaprolactone Scaffolds as a Drug Delivery System for 1,4-naphthoquinone Derivatives

Nadezhda V. Danilenko<sup>a\*</sup>, Evgeny N. Bolbasov<sup>a</sup>, Andrei I. Khlebnikov<sup>a</sup>, Igor A. Schepetkin<sup>b</sup> and Mark T. Quinn<sup>b</sup>

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## Abstract

Surgical resection of tumors often raises important problems of replacing and/or restoring lost tissue. To solve these problems, modern engineering suggests using polymer scaffolds as artificial porous structures. Possessing high biocompatibility, high strength, low degradation rate and the ability to release anticancer agents for a long time, polymer scaffolds made by electrospinning based on polycaprolactone (PCL) are one of the most promising types of scaffolds for restoring various types of tissues. One promising strategy for improving the properties of PCL scaffolds is loading low concentrations of effective anticancer agents into the scaffolds. This would facilitate production of PCL scaffolds with the required properties that take advantage of electrospinning technology.

Anticancer agents being considered for the development of PCL scaffolds are 1,4-naphthoquinone derivatives. Compared with known cytostatics, such as cisplatin, doxorubicin, 5-fluorouracil, some of these 1,4-naphthoquinone derivatives have higher anticancer properties.

In the present work, electrospun polycaprolactone (PCL) scaffolds doped with different levels of 2-chloro-3-((4-hydroxyphenyl)amino)-1,4-naphthoquinone (NQCP4) were fabricated without changing the technological parameters of the scaffold formation for the types of scaffolds that were tested. Loading NQCP4 into the spinning solution at concentrations of 10 to 50  $\mu\text{g}/\text{mL}$  did not cause changes in the structure, strength, and wettability of the scaffold. However, increasing NQCP4 contents in the spinning solution enhanced anticancer properties of the scaffolds *in vitro*. Such scaffolds could be used as promising materials with prolonged anticancer properties for tissue repair after surgical resection of tumors.

## Acknowledgement

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## Biodegradable and Injectable Poly (vinyl alcohol) Microspheres in Silk Sericin-based Hydrogel for the Controlled-release of Antimicrobials: Application to Deep Fullthickness Burn Wound Healing

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### Abstract

Deep full-thickness burn wounds are prone to multi-drug resistant (MDR) infections following injury, which extends the healing time. Thus, providing a bioactive hydrogel dressing with prolonged antimicrobial activity and reduced dressing changes is quite desirable for accelerating burn wound healing and preventing scarring. To achieve this, we developed an injectable hydrogel based on silk sericin (SS), poly (vinyl alcohol) (PVA), and PVA microspheres (MSs) containing vancomycin (VA), gentamicin (GEN), or their association (VG) for the healing of infected burn wounds. The microspheres were prepared by inverse emulsion crosslinking, while the hydrogels were prepared by freeze-thawing cycles. Antibacterial studies showed that gentamicin acts synergistically with vancomycin by increasing the bacterial killing rate and enhancing the biofilm inhibition and eradication effects on methicillin-resistant *Staphylococcus aureus* more than on *Pseudomonas aeruginosa* and *Escherichia coli*. Findings from SEM images showed that the microspheres were sphere-shaped with a smooth surface and their average diameter ranging from 26.22 to 32.42  $\mu\text{m}$  suitable for parenteral drug delivery. The prepared hydrogel containing 10% of microspheres was more elastic than viscous, with lower tan delta values ( $<1$ ) suited for deeper injection with homogeneous tissue integration. The incorporation of VG-PVAMS in the PVA/SS hydrogel led to zero-order release kinetics and efficient antimicrobial effects. Moreover, the *in vivo* study using a rat full-thickness burn model showed that the VG-PVAMS@PVA/SS hydrogel displays a better therapeutic effect than drug-free PVAMS@PVA/SS hydrogel and Tegaderm<sup>TM</sup> film dressing by inducing early vascularization and collagen deposition, leading to early re-epithelialization and burn wound closure.

## Fibrillated Bacterial Cellulose Liquid Carbene Bioadhesives for Mimicking and Bonding Oral Cavity Surfaces

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## Abstract

Topical treatments for oral wounds and infections exhibit weak adhesion to wet surfaces which results in short retention duration (6–8 hours), frequent dosing requirement and patient incompatibility. Mucoadhesive drug delivery platforms composed of Bacterial cellulose (BC) and photoactivated carbene-based bio-adhesives are combined to yield flexible film platforms for interfacing soft tissues in dynamic, wet environments. The first platform consists of carbene bio-adhesive layered onto dry BC matrix and is referred to as layered composite. The layered composite has an adhesion strength ranging from 7–17 kPa and duration exceeding 48 hours in wet conditions under sustained shear forces, while other mucoadhesives based on hydrophilic macromolecules exhibit adhesion strength of 0.5–5 kPa and last only a few hours. Second platform consists of aqueous composites made of fibrillated bacterial cellulose and photoactive bio-adhesives with uniform distribution of BC and carbene bio-adhesive. The composites crosslink upon photocuring within a minute and exhibit transition from viscous to elastic adhesive hydrogels. The third design, for the first time, presents dry, shelf-stable cellulose patches for convenient ready-to-use application. The dry patches simultaneously remove tissue surface hydration while retaining carbene-based photocuring and offers on-demand adhesion. The adhesion strength is higher than commercial denture adhesives on soft mucosal tissues. The structural integrity is maintained for a minimum of 7 days in aqueous environment. The patches act as selective nanoporous barrier properties against bacteria while allowing permeation of proteins. The results support the application of BC-based adhesive patches as a flexible platform for wound dressings, drug depots, or combination thereof.

## Session: Structural and Functional Materials

### Featured Presentations

#### Defects in an Orthorhombic MoAlB MAB Phase Thin Film

Rajib Sahu<sup>a,b\*</sup>, Dimitri Bogdanovski<sup>b</sup>, Jan-Ole Achenbach<sup>b</sup>, Jochen M Schneider<sup>a,b</sup> and Christina Scheu<sup>a,c</sup>

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#### Abstract

Tailored design of structural and functional materials always presents a challenge, with structural defects playing a significant role for material properties. Here, we report on the atomic-scale characterization of various coexisting multidimensional defects in a MoAlB MAB phase thin film by aberration-corrected scanning transmission electron microscopy (STEM). MoAlB, a ceramic nanolaminate, exhibits a combination of properties making it a promising candidate for various applications, such as use in protective coatings, as an oxidation-resistant material, conductor, battery electrode etc. MoAlB is also used as the precursor to synthesize the two-dimensional MBene MoB, usually via chemical etching, used in, e.g., energy research.

Here, we have grown an orthorhombic MoAlB thin film by direct current magnetron sputtering at 700 °C, a synthesis temperature reduced by approx. 42% compared to bulk synthesis approaches. STEM imaging reveals the formation of several defect types, such as 90°-twist boundaries, compositional defects (Mo<sub>3</sub>Al<sub>2</sub>B<sub>4</sub>), MoB side phase regions and 3D clusters, all coexisting in the MoAlB matrix. The presence of these defects is rationalized by the minute differences in their formation energies, as obtained from density functional theory calculations. In addition to MBene formation, Al deintercalation from MoAlB is observed at grain boundaries. This allows the conception of a straightforward MoB design route without using any chemical reagents, in contrast to prior approaches. Overall, we demonstrate the utility of advanced STEM imaging techniques (e.g. ABF, ADF, HAADF and iDPC) in guiding the design of MoAlB thin films at moderate temperatures.

## Self-Assembly of Chiroptical DNA-based Nanomaterials for Optoelectronic Technologies

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### Abstract

The universe is dissymmetric at all levels. Chirality is everywhere and on different levels from the subatomic to the macroscopic. Handedness is displayed by nature from chirality of atoms under the weak nuclear force to spiral galaxies, via countless examples such as amino acids, proteins, DNA, helical bacteria, helical plants, helical seashells, etc. DNA is one of the best naturally developed chiral systems, it offers astonishing capabilities for programmable, hierarchical, structure assembly with multi-dimensional and multi-material complexity. The robust nature of DNA and reliable synthesis associated with the ability to incorporate inorganic components addresses many of the criteria desired of a materials design toolkit. However, the combination of electrical conduction into the basic framework of duplex DNA remains challenging. Here, we demonstrate this with a sulfur-containing analog of a natural nucleoside (6-thioguanosine) that reacts with coinage metal(I) ions to spontaneously assemble circularly polarised luminescent (CPL), one-dimensional helical chains extending many  $\mu\text{m}$  in length. This DNA-like coordination polymer can be uniquely transformed into a wire-like conducting form by oxidative doping. With this, we advance the field of DNA-based materials toward further complexity by integration of semiconductive domains into DNA via self-assembly reaction of coinage metal(I) with a 6-thioguanosine-modified DNA duplex. These new types of compositional architecture and material combinations provides DNA-based materials with chiroptical semiconducting properties to make them as highly potential candidates for advanced optoelectronic technologies such as CP-OLED 3D displays, optical quantum computing and quantum communication, spintronics-based devices, security tags, biological probes and signatures, CPL lasers, CPL sensors, CPL-Spectroscopy and microscopy.

## Influence of the Laser Metal Deposition Process Parameters on the Structural Quality of a Cu-based Coating on Steel - A Preliminary Analysis

Federico Mazzucato<sup>a\*</sup>, Edouard Baer<sup>b</sup>, Francesco Impaziente<sup>a</sup>, Anna Valente<sup>a</sup> and Samuel Rey-Mermet<sup>b</sup>

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### Abstract

Metallic Functionally Graded Materials (FGMs) are advanced engineering solutions which exhibit unprecedented performance by taking advantage of the joining of dissimilar metals. Specifically, Copper-Steel bi-metallic structures are finding a growing application in industrial sectors such as Aerospace, Machinery, and Power generation, thanks to their enhanced wear/corrosion resistance combined with excellent mechanical properties. Nevertheless, the joining of Cu-based alloys on Steel still remains challenging due to the different coefficients of thermal expansion, the disparity in the melting temperatures, and diverse crystal structures. Powder-based Laser Metal Deposition (LMD) is an Additive Manufacturing (AM) technology that has demonstrated to have the potential to optimize FGM structures, enabling a more efficient functional part design. In this work, the authors characterise the deposition of a Cu-based alloy on a C45 Steel plate through powder-based LMD, achieving crack-free Cu-based coatings on Steel. The influence of laser power, axis speed, and plate preheating on the internal quality of linear single tracks is analysed, whereas the effect of the Oxygen content is assessed on the structural integrity of single circular layers. SEM and EDX analysis show defect-free clads and no diffusion of Steel into the as-deposited Cu-based material for specific energies ( $E_s$ ) ranging between  $60 \text{ J/mm}^2$  and  $17 \text{ J/mm}^2$ . On the contrary, at high energy densities ( $E_d$ ), the formation of both keyholes into the dilution zone and liquid metal embrittlement (LME) cracks into the Steel plate is encouraged. Moreover, crack-free single layers are achieved by reducing the content of Oxygen up to 1100 ppm during sample manufacturing.

## The Collective Friction and Wear Behavior of Tungsten Alloy Spheres

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<sup>b</sup>*Advanced Energy Science and Technology Guangdong Laboratory, China*

### Abstract

Granular matter can be extensively found in nature and industrial production. The granular flow spallation target composed of tungsten alloy balls, is considered as one of the promising candidate target types for the Accelerator Driven Subcritical System (ADS). Numerous target balls circulating in the target loop will cause strong and complex friction and wear, which will affect the service life of the target balls. So far, however, no suitable method and facility have been proposed to study and evaluate such the friction and wear behavior caused by the granular collective movement.

By using our self-developed device, we conducted the collective wear experiment of the tungsten alloy balls ( $\Phi$  1mm) at 250 °C under the protective atmosphere of helium gas.

It is found that the mass loss ratio of balls experienced six different states during the whole process. In the initial stage, fatigue wear is dominant, and then the micro-crack network on the surface of the ball begins to sprout and develops into a crushed layer. After the crushed layer falls off, the sub-surface begins to wear. Finally, a self-assembled new layer with a structure of amorphous surrounding nanocrystallines is formed on the ball surface. Moreover, the results also reveal the important roles of wear debris in different stages.

The results not only reveal some important characteristics of friction and wear behaviors among spherical granular during their collective movement for the first time, but also provide a crucial experimental method for evaluation of friction and wear behavior of the granular spallation target.

## Surface Induced Anti-foaming

Doris Vollmer\*, Katharina Hegner and William Wong

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### Abstract

Wet and dry foams are prevalent in many industries, ranging from the food processing and commercial cosmetic sectors to industries such as chemical and oil-refining. Uncontrolled foaming results product losses, equipment downtime or damage and cleanup costs. We show that passive defoaming or active anti-foaming is possible simply by the interaction of foam with chemically or morphologically modified surfaces. We tested superamphiphobic, liquid-infused and liquid-like surfaces using beer and aqueous soap solutions as model systems. Superamphiphobic surfaces are able to increase defoaming rates and inhibit foam formation (anti-foaming). They improved defoaming of highly stable wet foams and anti-foaming of growing dry foams. These improvements were quantified by monitoring the height of foam, the evolution of bubble numbers, radii, and coalescence-bursting events. Microscopic imaging reveals that amphiphobic nano-protrusions directly destabilize contacting foam bubbles. Bubbles burst, releasing gases through the Cassie-state's air-gaps. Interfacial destabilization of foam presents a new pathway for static defoaming and dynamic anti-foaming.

## Designing Self-cleaning Amphiphobic Coatings Based on Functional Acrylics

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## Abstract

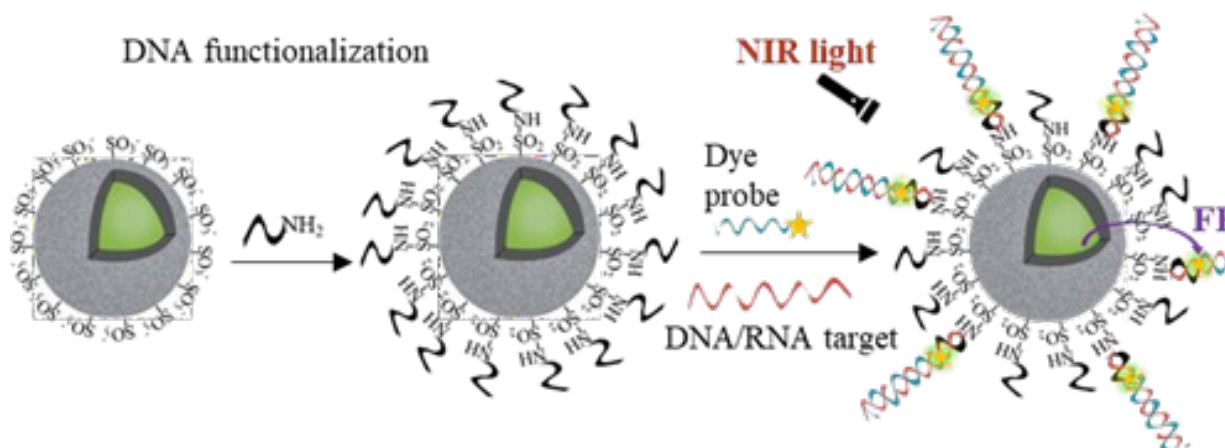
Self-cleaning or cleaning without manual intervention is desirable in coating industry as exterior facades are contaminated by dust and pollutants. We report the preparation of liquid repellent self-cleaning coatings using functional acrylic polymers via conventional radical polymerization. Both water based and solvent based random acrylic copolymers were prepared by emulsion and solution polymerization respectively. In this case, a solvent based single layer amphiphobic coating was prepared using principles of self-stratification. Low density glass hollow spheres and aerogel microparticles were used in designing this coating material. A robust two-layer coating with superhydrophobicity was also prepared using low cost microparticles. A water based near superhydrophobic coating was obtained using a combination of waxes with a styrene-acrylic emulsion. The solvent-based acrylics were crosslinked with 3-aminopropyltriethoxysilane while the water-based coatings were crosslinked with polycarbodiimide. Low contents of fluorinated components were used for the solvent-based coatings while the water-based coating was fluorine free. The coatings display the desired surface morphology and exhibit liquid repellency without the use of any nanoparticles. These coatings show potential applications as self-cleaning and easy cleaning coatings and can be applied by conventional means such as brushing and spraying.

## Near-infrared-based Sensitive Detection of Nucleic Acids with Upconversion Nanoparticles

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## Abstract

Upconversion nanoparticles (UCNPs) offer unique features for Förster Resonance Energy transfer (FRET)-based biosensing such as superior penetration depth and low biosample autofluorescence due to near-infrared (NIR) excitation, low cytotoxicity, high stability or absence of photoblinking or photobleaching. However, a proper surface modification with a recognition moiety is required in order to ensure not only high FRET efficiency but also the stability of the nanohybrid. In this work, we describe a novel and original method for the synthesis of a DNA-coated UCNPs probe for the detection of nucleic acids in a homogeneous assay. The designed nanoprobe displays high specificity and versatility since can be adapted for both DNA and RNA. Interestingly, the assay shows an extraordinary sensitivity reaching a limit of detection value as low as 45 fM for miRNA20a without any amplification strategy.



**Figure 1:** Illustration of the synthetic procedure of the nanohybrids and their nucleic acid-sensing performance.

## Acknowledgments

Authors thank the European Union's Horizon 2020 research and innovation programme (Marie Skłodowska-Curie Individual Fellowship 794410), Universitat de València (Subprograma Atracció de Talent Contractes Postdoctorals), COST Action CM1403 (The European Upconversion Network), the French National research agency (LaPin project ANR-20-CE09-0021-02), and Generalitat Valenciana (No. PROMETEO/2019/080).

## Use of Polymer Micropillar Arrays as Templates for Bioanalytical Assays

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### Abstract

We describe the use of periodic micropillar arrays produced by high-fidelity microfabrication with cyclic olefin polymers as substrates for colorimetric and fluorescence-based DNA and protein detection assays. These three-dimensional templates offer higher surface-to-volume ratios than two-dimensional substrates, making it possible to attach more analyte to the surface and so increase the signal obtained by the assay. Micropillar arrays also provide the capacity to induce wicking, which is employed to distribute and confine capture moieties on the surface with spatial control. The relationship between microstructure and assay response was investigated through variation of geometrical parameters such as pitch (10–50  $\mu\text{m}$ ), pillar diameter (5–40  $\mu\text{m}$ ), and pillar height (5–57  $\mu\text{m}$ ). Our findings reveal that assay response deviates from a linear relationship for colorimetric detection where the formation of color pigments interferes with diffusion and mass transport into the deeper portions of the wells. These observations are supported by a theoretical model used to simulate changes in surface composition at the molecular level, suggesting differences in the temporal and spatial accumulation of assay components across the array in the absence of flow. For fluorescence assays, on the other hand, a linear relationship between signal intensity and micro-scale structure can be maintained even when aspect ratio and pillar density become very high, opening the possibility of tuning assay response by design over a wide dynamic range compatible with different samples, analyte concentrations and readout instruments.

## Understanding Potential-driven Ion Separations at Solvated Electrified Interface

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### Abstract

Electrochemical separations are sustainable and efficient compared to chemical processes because of their lower energy costs, reusability, and ease of integration with available power sources. Selective adsorption of ions at electrochemical interfaces used in electro dialysis-based critical metals and minerals extraction can be modulated by non-Faradaic (capacitive) and Faradaic (redox) approaches. The hydrophobicity and solvent dipole at electrochemical interfaces play a key role in the partitioning of metal ions from the bulk solution region and facilitate stable and selective transport and adsorption of targeted ions at interfaces. The main objective of our research is to enable predictive understanding of the factors influence the separation of solvated targeted metal ions (e.g., Pb, Cd, La, Eu, Yb) by modulating the interfacial solvation dynamics and potential energy profile through surface functionality, hydrophobic domains, and electric fields. Herein, we will present our recent developments to modulate desolvation and selective adsorption dynamics at well-defined electrochemical interfaces by functionalizing electrodes with task-specific ionic liquid cluster ions (e.g., 1-n-alkyl-3-methylimidazolium cations  $[\text{C}_n\text{mim}]^+$  and multi-electron redox-active polyoxometalate (POM) anions to impart a different degree of hydrophobicity and Faradaic adsorption/reduction at the electrified interface, respectively. We established the structure-function relationship between charged IL cluster  $[\text{C}_3\text{mim}]_n[\text{BF}_4]_{n+1}^-$  ( $n=1-9$ ) anions, POM anions and targeted metal ions at the interface using combined experimental and theoretical approaches such as ion soft landing, *in-situ* infrared reflection-absorption

(IRRAS) and Raman spectroscopy and advanced machine learning level theoretical simulation, which enabled to prepare, characterize, and model the well-defined electrochemical interfaces towards separation of critical metal and minerals.

## **Ranking of Factors Influencing the Construction Waste Generation in Construction Companies of a Defined Size**

**Marta Bialko**

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### **Abstract**

The subject of the analysis is the ranking of factors that affect the construction waste generation in construction companies and its dependence on companies' size. The research was based on 140 surveys conducted in Sharjah, in the UAE among construction companies. Factors influencing the construction waste generation were divided into those occurring in the design phase (10 factors) and construction phase (8 factors) of a building, as well as related to the management of construction products (8 factors) and work culture (4 factors). The methodology was divided into two parts: (1) to rank the factors, the measure of central tendency and dispersion was examined using the mean, median, standard deviation, minimum, maximum and skewness, (2) to examine the dependence of the assessment of the impact of factors on waste generation on the size of the company, the statistics of the Kruskal Wallis test with the Dunn's post hoc test were calculated. The analysis of the ranking of all factors shows that factors related to work culture were rated the highest and factors related to product management were rated as having the lowest impact on waste generation. The statistically significant difference in the assessment of the factors' impact on waste generation depending on the size of the company was confirmed for 19 factors out of 30 examined. Based on the results of the conducted research, it can be concluded that raising awareness of the negative impact of waste on the environment, and thus having a waste management plan, can have a significant impact on reducing the amount of construction waste by, among other things, choosing products with high quality, and training employees in the field of construction waste management.

## **Young Researcher Presentations**

### **The Influence of Construction Waste from Concrete on the Alkaline Activation Process of New Fly Ash-based Geopolymer Construction Materials**

**Felix Kugler<sup>a\*</sup>, Wolfgang Krcmar<sup>b</sup> and Ulrich Teipel<sup>b</sup>**

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*<sup>b</sup>Department of Chemical Engineering, University Ulm, Germany*

### **Abstract**

The construction industry is at the same time one of the biggest economic factors, but also one of the biggest polluters of the environment, which is why new "green" building materials have to be developed quickly. One of the hopefuls are alkaline activated materials or geopolymers. These two classes of materials are based on the same manufacturing process, alkaline activation, but differ slightly in their chemistry and resulting properties. Therefore, our work investigated blends of fly ash-based geopolymers and alkaline-activated concrete rubble-based materials. Geopolymers form well cross-linked sodium silicate hydrates and alkaline activated materials form less well cross-linked calcium aluminosilicate hydrates. These studies will help to better understand the interactions of the two different setting processes on each other, to elucidate the material properties resulting from mixing and thus to open up new raw material sources for alkaline activation. The setting behavior and the forming structures will be

investigated by infrared spectroscopy, X-ray diffraction analysis and scanning electron microscopy. In the course of the investigations, the manufactured geopolymer samples are examined for the material parameters relevant to building materials, namely compressive strength, bulk density and thermal conductivity. Thus, the highest compressive strengths measured were  $\sigma_d = 113$  MPa, the lowest density was  $\rho_{roh} = 1.69$  gcm<sup>-3</sup>, and the lowest thermal conductivity was  $\lambda_{10,dr.} = 0.354$  Wm<sup>-1</sup>K<sup>-1</sup>.

### Acknowledgment

The research leading to these results was funded by the European Union through the LIFE Program 2014-2020 for Environment and Climate Action under project number LIFE18 CCM/ES/001114.

## Investigation of Ceramics Matrix Composite Material Suitability for an Aeronautical Application

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<sup>c</sup>*Eukasiewicz Research Network – Institute of Aviation, Poland*

### Abstract

In the aerospace field the introduction of innovative materials has been of crucial importance to reduce weight and to increase performances and safety. Ceramics Matrix Composites (CMC), which over the years they have become more commonly used due to the implementation of more cost-effective production methods, allowed to design and produce lightweight structures with load carrying capabilities at extremely high temperatures. This work aims to redesign an aeronautical exhaust muffler, currently produced using metallic materials, employing CMC material, which will improve the thermal and noise abatement performances while complying to stringent requirements in terms of weight and fire resistance. The material was subjected to different mechanical tests aiming to characterize its properties and to define design values for the verification of the structure. Moreover, due to the projected application the tests were performed both on virgin and on oxidated specimens. The tests highlighted a particular response of the material, which is characterized by a pseudo-plastic behavior, and demonstrated that the material is capable of resisting to high temperature in an oxidizing atmosphere for long times. Finally, the component was not designed from scratch, but part of the solutions adopted followed the current design philosophy, thus leading to the need to laminate complex shapes. The technological trials performed on these shapes showed undesirable distortion in the element associated to the production process and a possible approach to numerically predict this phenomenon is outlined, aiming to implement solutions to compensate the undesired effects.

## Effect of Cold Forging on the Evolution of Microstructure and Texture in Beta-C Titanium Alloy

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### Abstract

A single-phase Ti-3Al-8V-6Cr-4Mo-4Zr (Beta-C) titanium alloy was directed to uniaxial compression at room temperature. The microstructural evolution during uniaxial cold compression was studied using field emission scanning electron microscopy, and electron backscattered diffraction, while, X-ray diffraction was performed to measure bulk crystallographic texture. Significant increase in stored energy induced peak broadening at higher deformation. The texture evolution during cold compression was simulated using mean-field Taylor models (MTM-TAY). The deformed microstructure (after 45% compression) exhibits prominent shear bands, preferentially in

compression direction, that is CD//<111> oriented grains. CD//<100> fiber and CD//<111> fiber were the most prominent crystallographic texture components created during compression. With increasing compression, a subtle shift in texture was detected. The full constraint Taylor model revealed a reasonable agreement between simulated and experimental texture.

## Strengthening the Re-free Second-generation Single Crystal Superalloy by Constructing $\gamma/\gamma'$ Phase Interface with Low Energy

Xipeng Tao\*, Xinguang Wang, Jinguo Li, Yizhou Zhou and Xiaofeng Sun

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### Abstract

The sustainable development of nickel-base single-crystal (SX) superalloy is seriously restricted by over alloying. However, low alloying could significantly reduce the  $\gamma$  and  $\gamma'$  phases strength and the  $\gamma/\gamma'$  phase interface stability in SX superalloys. In this study, the stable  $\gamma/\gamma'$  phase interfaces with low energy were designed and constructed in a novel Re-free second-generation SX superalloy by tailoring composition. The chemical contents of  $\gamma'$ -forming elements (Al+Ti+Ta) were designed as 6-15wt%, which guaranteed the specific surface area of  $\gamma'$  phase up to  $1.2 \times 10^4 \text{ cm}^2/\text{g}$ . Meanwhile, the Re, Mo and Cr elements were replaced by Co, W and Ta elements in the novel superalloy, which reduced  $\gamma/\gamma'$  phase interface energy by 30%. The stable  $\gamma/\gamma'$  phase interfaces significantly retarded the  $\gamma'$  phase rafting rate and increased the density of  $\gamma/\gamma'$  phase interfaces dislocation network during high-temperature creep test. The novel Re-free SX superalloy strengthened by constructing  $\gamma/\gamma'$  phase interface with low energy exhibited the similar ultimate tensile strength, high-temperature creep life and high-cycle fatigue life to the traditional Re-containing second generation SX superalloys. This research provided an advanced and revolutionary technology to greatly reduce the dependence of SX superalloys on rare and precious metal resources, and realize the transformation of high-performance SX superalloy development from over alloying to plainification of alloying.

## Revealing Oxidation Mechanisms of TiAlN Coatings Inside Oxygen-saturated Lead-Bismuth Eutectic

Essam Serag<sup>a,b\*</sup>, Emile Haye<sup>a</sup>, Ben Caers<sup>b</sup>, Paul Schuurmans<sup>b</sup> and Stéphane Lucas<sup>a</sup>

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<sup>b</sup>*Belgian Nuclear Research Centre (SCK•CEN), Belgium*

### Abstract

Lead bismuth eutectic (LBE) will be used as a liquid metal coolant in accelerator driven systems such as MYRRHA. LBE is a corrosive medium, especially at elevated temperatures, jeopardizing the integrity of the exposed materials. The situation is even more challenging for mechanical components (e.g. journal bearings) of the in-vessel fuel handling systems that operate inside LBE, this is due to the inability of LBE to act as a lubricant layer promoting surface friction and wear. Many studies proved the ability of TiAlN coatings to protect surfaces against wear and corrosion at high temperatures in air. Ti<sub>0.46</sub>Al<sub>0.54</sub>N coatings have been deposited on AISI 316L substrates using reactive magnetron sputtering technique. The coatings' properties were first investigated varying the deposition parameters to identify the optimum conditions in which coatings with high hardness, low residual stress and high toughness are achieved. Deposition done at 100V and 5mTorr develop coatings with high hardness ( $\approx 38 \text{ GPa}$ ) and moderate compressive residual stress ( $\approx 2.84 \text{ GPa}$ ). The optimized coated samples were then immersed in static oxygen-saturated LBE to understand their oxidation mechanisms. The tests took place in LBE at 250°C and 360°C for 500h and 1000h, and at 410°C for 500h. XPS depth profiles show no oxidation taking place at 250°C even after 1000h. However, an oxide layer consisting of Al<sub>2</sub>O<sub>3</sub>+TiO<sub>2</sub> was formed on the surface of the coating at 360°C, while an oxide bilayer (TiO<sub>2</sub> / Al<sub>2</sub>O<sub>3</sub>+TiO<sub>2</sub> depleted of Ti) of thickness 285nm was formed at 410°C after 500h. An oxidation mechanism is proposed based on the results.

## Poster Presentations

### 3D Printing Technology for Green Construction

**Guilherme Pante Leme de Campos<sup>a</sup>, Pietro Sinigaglia Lunelli<sup>a</sup>, Marcelo Tramontin Souza<sup>a,c</sup>, Elisângela Guzi de Moraes<sup>a,b</sup> and Antonio Pedro Novaes de Oliveira<sup>a\*</sup>**

<sup>a</sup>Laboratory of Glass-Ceramic Materials (VITROCER), Department of Mechanical Engineering, Federal University of Santa Catarina (UFSC), Brazil

<sup>b</sup>Department of Automation and Systems, Graduate Program in Automation and Systems Engineering (PosAutomação), Federal University of Santa Catarina (UFSC), Brazil

<sup>c</sup>Laboratory of Mechanical Tests and Resistance of Materials (LEMER), Department of Exact and Technological Sciences, State University of Santa Cruz (UESC), Brazil

#### Abstract

The present study aims to test ceramic pastes by 3D printing using natural materials such as clays and plant fibers, designed for printing biohouses. Clays with different characteristics were explored, changing the contents of water (29 to 80 wt.%) and fibers (sugar cane bagasse, 1 to 2 wt.%) present in the composition. The materials were homogenized in a mechanical stirrer and subsequently tested for printability (extrudability) and buildability (number of printed layers). Simultaneously, the extrusion pressure was monitored and after printing, the drying shrinkage was evaluated with an analogic caliper of the printed components after seven days of drying at room temperature. It was found that water plays a key role in the workability and shrinkage of materials. The compositions with higher water contents operated in a lower pressure range (below 1 bar) and achieved considerable shrinkage rates (>40%). Fiber, on the other hand, decreased the drying shrinkage of the printed components (<7%) but increased the required working pressure (2.5 bar).

### Additive Manufacturing of Recycled Soda-lime Glass Structures

**Antonio Pedro Novaes de Oliveira<sup>a\*</sup>, Elisângela Guzi de Moraes<sup>a,b</sup>, Igor Maia Ferreira<sup>a</sup>, Luyza Bortolloto Teixeira<sup>a</sup> and Marcelo Tramontin Souza<sup>a,c</sup>**

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#### Abstract

Additive manufacturing (AM) technology has shown great potential due to its versatility, allowing the fabrication of custom-shaped, dense or porous structures, through layer-by-layer deposition. The technical feasibility of AM depends on a rigorous control of the rheological properties of printing inks, which needs to have pseudoplastic flow behavior, i.e., fluidity for pumping and plasticity for extrusion/printing, while at the same time be able to support the weight of the overlapping layers. The aim of this work is to produce cellular glass structures by direct printing (robocasting) using bentonite to supply the lack of plasticity of glass powders. Ceramic inks containing recycled glass powders ( $d_{50} < 4 \mu\text{m}$ ) and bentonite (6.5 to 9.5 wt.%) were previously mixed and printed using a 1.60 mm printing nozzle at a 10 mm/s printing speed. The three-dimensional structures were dried at room temperature for 24 h and then fired at 700 °C for 1 h at a heating rate of 10 °C/min. The components obtained from recycled glass showed porosities of up to 53%, pore sizes between 1090 and 1870  $\mu\text{m}$  and compressive strength of about 18 MPa.

## Nanocrystalline Coatings for Filtration Applications

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### Abstract

Filtration technologies are of the highest interest for the human civilization. They decrease the air pollution and ensure wide access to drinking water. Filtration plays important role also in chemical and food industries, where limitation of bacteria growth and reemission of microorganisms is one of the key factors to extend the lifetime of a filter membrane. It can be realized by deposition of appropriate materials on the filter surface. However, such operation cannot disturb the flow of media through the membrane. At the first stage of the work, nanocrystalline coatings composed of CuO, AgO and AgO+CuO were deposited on model Si substrate. The influence of cathode (Cu or Ag) power (in the range between 50–200 W) on coating thickness, surface morphology, microstructure and chemical composition was analyzed. In the second stage, selected coatings were deposited on the filter membranes. The distribution of the deposited material on the membrane surface was analyzed.

The investigation evidenced that the obtained coatings were characterized by homogeneous, nanocrystalline structure. However, CuO and AgO coatings differ in microstructure and morphology. CuO coatings exhibit columnar or needle like structure, while nano-grains in AgO coatings have more equized shape. Moreover, in case of multicomponent coatings (AgO+CuO), changes in the cathode (copper or silver) power results in differences in coating microstructure. The use of two sources leads additionally to composite structure (matrix and fine particles) of the coating.

## Nanostructured Gadolinia Doped Ceria Ceramics for Low-temperature Solid Oxide Fuel Cells Application

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Kaunas University of Technology, Lithuania

### Abstract

One of the most frequently studied and used electrochemical energy conversion devices are solid oxide fuel cells (SOFCs). Low-temperature SOFCs (LT-SOFCs), operating at 400–650 °C, are denoted by a shorter start-up time, do not require expensive materials, and can be used in portable devices. Gadolinia doped ceria (GDC) is still one of promising electrolyte material for LT-SOFC application. Due to their chemical stability and high ionic conductivity, GDC ceramics can be used not only as an electrolyte, but also as a diffusion barrier layer between the cathode and electrolyte in SOFCs. In this work, GDC nanopowders were synthesised by co-precipitation synthesis method and used as a target material to form ceria-based thin films using the electron-beam evaporation technique. The morphological properties of the pressed ceramic pellets were examined using scanning electron microscopy (SEM). The impedance spectroscopy showed an increase in the total resistance of ceramics with the increase of the concentration of Gd<sub>2</sub>O<sub>3</sub> in GDC. The annealing of the GDC films up to 900 °C had a minor affects its surface roughness and the morphology with minimal increase of the densification and roughness. XRD and Raman spectroscopy results confirmed the improvement of the crystallinity for corresponding thin films and the decrease of grain boundary phase volume. XPS and ICP-OES measurements showed that, to obtain the desired concentration of the final thin films, the concentration of the synthesised target material used for the electron beam evaporation should be ~28 % higher.

## Using Anionic Surfactants to Study Removal of Alkanes from Dolomite and Graphite Surfaces: A Molecular Dynamics Study

Hector Dominguez\* and Ana Beatriz Salazar-Arriaga

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### Abstract

Hydrocarbon pollution is an important issue in different environmental problems, so in this work we study a computational model to investigate the removal of contaminants from solid surfaces by means of surfactants molecules. Using Molecular Dynamics techniques, we conducted simulations of sodium dodecyl sulfate (SDS) surfactants on graphite and dolomite surfaces contaminated with a mixture of several alkanes at different compositions. Then, desorption studies of alkanes from the plates were carried out at distinct SDS concentrations with and without the presence of electric fields. Positive and negative electric fields of different intensities were tested, and it was noted that the positive fields promote detachment of the alkane molecules however, complete removal is obtained with the negative high electric fields. Analysis was conducted in term of density profiles and adsorption isotherms.

### Acknowledgement

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## Residual Stress Map for 75Ni13.5Cr2.7B-3.5Si Clad 316 Stainless Steel

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### Abstract

Plasma Transferred Arc (PTA) process uses the intense heat of electric arc to melt and fuse the 75Ni13.5Cr2.7B-3.5Si hard-facing alloy and the base metal. This process develops substantial residual stresses near the hard-faced surfaces during deposition and subsequent solidification and cool down. Furthermore, when a material interface is present, additional residual stress is formed because of the thermal strain mismatch of the dissimilar materials caused by their different thermal expansion coefficients. These stresses can cause cracks in the overlay during the component's service life or even earlier during manufacturing which can lead to partial or total loss of the part structural integrity. To start optimizing the process to avoid these defects, it is necessary to know the residual stress distribution in the part and how it is related to the process parameters. Hard-faced components are having distinct microstructures with a step change in material properties, and this makes the residual stress measurement more challenging. This paper presents 2D residual stress maps of the deposit cross sections for PTA hard-faced samples using the contour method. This study is part of an ongoing research on the influence of process parameters on the residual stress and local microstructure of 75Ni13.5Cr2.7B-3.5Si clad 316 stainless steel.

## Synthesis of Er Doped Gold Nanoparticles by Laser Ablation in Water: A Fundamental Study of the Exchange Interaction Between Localized Magnetic Moments and Conduction-electrons

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## Abstract

In this work we report the synthesis of  $\text{Au}_{1-x}\text{Er}_x$  ( $x \leq 0.026$ ) nanoparticles (NPs) produced by pulsed laser ablation starting from alloy targets submerged in deionized water. A fundamental study on the exchange interaction between localized rare earth magnetic moments and conduction-electrons of  $\text{Er}^{3+}$  diluted in Au metallic NPs is given. The study was carried out in  $\text{Au}_{0.992}\text{Er}_{0.008}$  and  $\text{Au}_{0.974}\text{Er}_{0.026}$  bulk metallic alloys and NPs. The samples were characterized by means of X-ray diffraction, transmission electron microscopy, magnetic susceptibility and electron spin resonance (ESR) experiments. The structural results shown that the NPs produced by laser ablation have spherical shape with middle size of 20 nm and large size dispersion. The magnetic results showed that, despite the high temperature and far away from chemical equilibrium throughout the laser ablation process, the  $\text{Er}^{3+}$  ( $J=15/2$ ) ground state of the crystal electric field splitted multiplet remains a  $\Gamma_7$  ( $g=6.79$ ) Kramers doublet with the expected  $g$ -shift and  $T$ -dependence of the ESR linewidth, preserving the general bulk properties and the cubic symmetry. Besides, the  $\text{Au}_{1-x}\text{Er}_x$  NPs present narrow ESR residual linewidth suggesting homogeneous  $\text{Er}^{3+}$  doping and negligible strain distribution in the NPs. We believe that this report may open new window to explore the fundamental physics properties in other rare-earth doped metals, intermetallic or semimetals nanomaterials with different morphologies by the "top down" laser ablation route, as well as novel technological applications at the nanometer scale.

## Effects of Morphology, Magnetism and Composition on the Magnetic Fluid Hyperthermia Response of $\text{Co}_x\text{Fe}_{3-x}\text{O}_4$ Nanoparticles for Use as a Drug Carrier

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### Abstract

In this work, we present a study of the morphological and magnetic properties of  $\text{Co}_x\text{Fe}_{3-x}\text{O}_4$  nanoparticles to understand their magnetic fluid hyperthermia (MFH) response. By controlling the size and the composition of our samples we tune the effective magnetic anisotropy and the saturation magnetization, which allow us to optimize the SPA (specific power absorption) of our material in MFH experiments. NNPs with sizes between 9-12 nm were synthesized by high temperature thermal decomposition of organometallic precursors. The crystal structure, chemical composition and morphology of the nanoparticles was determined by X-ray Diffraction (XRD), Transmission Electron Microscopy (TEM) and Electron Scattering Spectroscopy (EDS) measurements and the magnetic properties were determined by magnetization measurements. The magnetic hyperthermia experiments were performed as a function of concentrations of the MNPs, frequency, between 100kHz and 575kHz and amplitude up to 56mT, in two different rheological conditions (different viscosities). The resulting SPA values were analyzed in terms of the different mechanisms that determine the magnetic losses. These mechanisms are related to the magnetic relaxation of the nanoparticle's moment and its phase shift respect to the ac applied field I show that the result of the SPA does not change by varying the concentration from 0.5mg/mL to 5.2mg/mL and varying the medium with low viscosity and high viscosity, being an indication that the MNPS heat up by the Néel relaxation mechanism. Mechanism of interest for the use of a drug carrier, based on liposomes.

## Reversible Mono- and Dual-metal Ion Intercalation into Alkali Transition Metal Sulfates in Different Electrolytes

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### Abstract

Polyanionic compounds belong to the main class of electrode materials for both lithium- and sodium-ion batteries that respond, to a great extent, to the modern requirements for efficient, safe and environmental compatible storage

of energy. Among polyanionic compounds, sodium transition metal sulphates attract considerable interest as low-cost electrode materials offering high operating voltage for alkaline ion intercalation.

In this contribution we demonstrate for the first time the reversible electrochemical intercalation of Li<sup>+</sup>/Na<sup>+</sup> ions into A<sub>2</sub>Mn<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> (A = Li, Na) as a positive electrode in alkali-ion cells. Sulfate salts were simply obtained by thermal dehydration of the respective hydrate or lyophilised precursor. The mono- and dual-ion intercalation into the sulfates was examined in model electrochemical cells by using Li/Na metal as a negative electrode and in presence of carbonate- and ionic liquid-based electrolytes. The cycling voltammetry experiments were carried out at room and elevated temperatures. A mechanism of the electrochemical reaction is monitored by *ex-situ* analysis.

### Acknowledgement

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## Structural Modeling of Layered Na<sub>2/3</sub>Ni<sub>1/2</sub>Mn<sub>1/2</sub>O<sub>2</sub> Oxide via Selective Substitution for Ni<sup>3+</sup> with Al<sup>3+</sup> Ions

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### Abstract

The sodium transition metal oxides with layered structure are among the most promising positive electrode materials for sodium-ion batteries. However, these types of oxides have not yet reached their optimal electrochemical properties in terms of specific capacity and cycling stability.

Herein we provide new data on the structural modeling of layered Na<sub>2/3</sub>Ni<sub>1/2</sub>Mn<sub>1/2</sub>O<sub>2</sub> (0 ≤ x ≤ 1/6) oxides via selective substitution for Ni<sup>3+</sup> with Al<sup>3+</sup> ions. It was found that the presence of aluminum ions in the layered oxide leads to the formation of a mixed P3-P2 type of structure. The ratio between P3-P2 phases depends on the synthesis temperature: at low temperature is dominating the P3-phase, while the P2-phase become more dominant with increasing the temperature. The electrochemical tests are carried out in model cell versus Na metal and in conventional 1 M NaPF<sub>6</sub>:PC electrolyte. It is discussed the specific capacity and cycling stability of Na<sub>2/3</sub>Ni<sub>1/2-x</sub>Al<sub>x</sub>Mn<sub>1/2</sub>O<sub>2</sub> oxide in terms of synthesis temperature, respectively correlation between electrochemical properties and P3-P2 phases ratio.

### Acknowledgement

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## Structural Materials Used for Ecological Restoration of Damaged Ecosystem Based on Biomimicry Concept

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### Abstract

Biomimicry concept should extend to new fields, so we think it's an effective approach that can restore the alpine environment. *Abies koreana*, endemic in Korea, have been afforested. But now it should be restored using ecological methods. To do this, we need a view point of ecological restoration by biomimicry. First, we elucidate a mitogenome structure (1.1 Mb & 59 genes). Through this, *Abies* spp. can be distinguished and determined the appropriate genotype. Second, a restoration structure is invented. This technology can settle young seedlings of alpine conifer. When an alpine conifer falls due to strong winds, seeds drop on the fallen trees and young seedlings grow. This is

called “regeneration on fallen dead trunk”. So we mimic this phenomenon. By using this, seedlings can grow without disturbance, and even if the structure is decomposed, it doesn't have a negative impact on the ecosystem, rather, it can be used as nutrients. Third, endophyte having an antifungal function was selected and inoculated aseptically into seedlings. Particularly, this fungus can control damping off disease, which is a major hindrance to the initial growth of seedlings. Fourth, in order to install the inoculated seedlings and structures, we try to make a model to anticipate an optimal points that can spread the seeds from *Abies koreana*. Approaches to environmental challenges can be obtained mainly by understanding each factors affecting the network. This study shows a possibility that biomimicry thinking can make a closed circular model through the understanding of gene, seed, and succession mechanisms etc.

## Ag Nanoparticles-Doped Poly(ether ether ketone) for Potential Use in Biomedical Applications

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### Abstract

Polymeric materials are currently widely used materials in the fields of bioapplications and tissue engineering. As they seldom meet the strict requirements for applications, a solution can be found in their surface treatment. A promising technique today is surface laser modification, which under specific conditions can lead to the formation of a nanostructured surface. The resulting structures then allow for better adhesion of the cells to the surface or provide space for further surface treatments, namely the deposition of metallic materials. This work represents the surface treatment of polyethylene naphthalate by irradiation with KrF excimer laser and subsequent deposition of Au nanowires using the vacuum evaporation technique. The surface morphology varied depending on the incidence angle of the laser beam, which was observed by AFM and SEM analyzes. XPS was used to confirm the presence of Au nanowires and to determine the surface composition of samples. Finally, drop plate antibacterial and cytotoxic tests were performed to determine the role of Au nanowires important for the use of the resulting composite in bioapplications.

## Plasmon-assisted Functionalization of MXene Surface

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### Abstract

A new class of materials, MXenes, are a family of two-dimensional (2D) transition metal carbides, carbonitrides, and nitrides with the general formula  $M_{n+1}X_nT_x$ , where  $n + 1$  ( $n = 1-4$ ) - layers of early transition metals (M), X is an element such as carbon or nitrogen,  $T_x$  in the formula represents the surface terminations, such as O, OH, F, and/or Cl, which are bonded to the outer M layers. MXene has plasmon-active properties, which allows us to introduce an interesting new concept in the chemistry of materials - the utilization of plasmon assistance to activate a chemical transformation. This approach can be used for nano-precise and spatially selective surface grafting of plasmon-active nanomaterials. In the case of MXenes, the possibility of plasmon grafting is particularly attractive, since the properties of MXenes are strongly determined by their surface-terminated groups. To date, known methods for modifying the surface chemistry of MXene flakes rely on high-energy treatments (e.g., high-temperature annealing) and often result in damage to the MXene structure.

In this work, we demonstrated a modification of  $Ti_3C_2T_x$  flakes, based on plasmon-activation of iodonium salt, the subsequent creation of highly reactive radicals, and their immediate grafting to flakes' surface. The ability of  $Ti_3C_2T_x$  surface chemistry tuning (i.e., grafting of organic groups with various substituents) opens new possibilities for this material application.

## Development of Glioblastoma-homing and H<sub>2</sub>O<sub>2</sub>-Responsive Therapeutic Prodrug

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### Abstract

Glioblastoma (GBM) is the most common primary malignant brain tumor in adults, accounting for 16% of the primary malignant tumor of the central nervous system. At present, chemotherapy is the most successful method to treat GBM. However, low GBM-targeting ability and penetration efficiency could induce several side effects.

In this study, we developed a new GBM-homing and in situ activating-therapeutic material to address the issues. This therapeutic prodrug consists of a specific peptide, in situ responsive part, and an anti-GBM drug. The therapeutic prodrug entered into GBM cells via over-expressed receptor-mediated endocytosis. In the GBM site, the material was in situ activated by intracellular reactive oxygen species (ROS) and released free anti-GBM drug. We demonstrate the applicability of GBM-targeting and in situ activating therapeutic materials in GBM cancer cells (U87MG) comparing other cancer cells, and it showed a higher therapeutic efficacy through hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>)-induced drug activation and drug-induced cell death. This study presents a new strategy for the development of efficient GBM treatment using over-expressed intracellular H<sub>2</sub>O<sub>2</sub>. We expect this therapeutic material to reduce the side effects of chemotherapy and contribute to the treatment of GBM.

## Generation and Characterization of Core-Shell Microparticle Containing Water Core for Biomedical Purposes

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### Abstract

Core-shell microparticles have emerged as a promising device for biomedical purposes, including regenerative medicine, tissue engineering, and targeted delivery of therapeutic agents. The essential step in producing such a unique-structured microparticle is forming a droplet template. Herein, we present a facile technique to produce a surfactant-free core-shell droplet with a water core using a flow-focusing microfluidic device. The solid microparticles were obtained by polymerizing the droplet's polymeric shell of trimethylolpropane trimethacrylate (TMPTMA). The microfluidic technique enabled precise adjustment of the core and the shell geometries by changing the flow rates of the components. Optimized single core-shell microparticles had a core and a shell radius of about 30 μm and 60 μm, respectively. In the next step, we studied experimentally and analytically the behavior of resultant microparticles under thermal and mechanical loads. Three different microparticles with the ratios of the shell thickness to the outer radius  $T_{\text{Shell}}/R_{\text{Core-Shell}}$  of 0.37, 0.41, and 0.46 were investigated, respectively. The compression test results revealed that the resistance of microparticles to deformation and rupture increases by increasing  $T_{\text{Shell}}/R_{\text{Core-Shell}}$ . The critical rupture displacement of the microparticles scales directly with  $T_{\text{Shell}}/R_{\text{Core-Shell}}$ . The results implied that microparticles' average critical rupture temperatures are independent of  $T_{\text{Shell}}/R_{\text{Core-Shell}}$ , and all rupture at about 113 °C. Microparticles' thermal and compression responses were then compared with the existing predictive models. The results indicated that the predicted behaviors of the microparticles agree well with the experimental data. Water- TMPTMA core-shell microparticles showed considerable thermal and mechanical stability critical for biomedical applications such as bioreactor and bone and cartilage tissue engineering.

## Porous Silicon Surface Functionalization via Microwave-induced Si-S Bond Formation

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### Abstract

Porous silicon (pSi) materials have received attention due to several advantages such as high biocompatibility, high drug-loading capacity, intrinsic photoluminescence property, and high applicability via additional surface modifications. Therefore, pSi materials are preferred in diverse chemical, biological, and medical fields. In this vein, various surface functionalization methods have been developed for these purposes. Among the functionalization methods, a hydrosilylation reaction that uses hydrogen from the pSi surface is a well-known method. This reaction can be progressed by diverse energy sources such as heat, light, and microwave. However, this reaction should have occurred under the inert gas condition because an un-oxidized surface of pSi is required.

This study disclosed an efficient and straightforward surface modification method that makes covalent Si-S bonds on the hydrogen-terminated (H-terminated) surface of pSi using a microwave. This chemistry is promoted by the ring-opening of the cyclic disulfide compound, and then it forms Si-S covalent bonds on the pSi surface. Surprisingly, it takes less than 10 minutes, and this is a more efficient and helpful method than any other commonly used methods (e.g., ultrasonication, heating stirrer, and vortexing) when analyzing with the scanning electron microscope (SEM), energy dispersive spectrometer (EDS), attenuated total reflectance Fourier-transform infrared (ATR-FTIR), and water contact angle analysis. We demonstrated this on a pSi wafer, pSi rugate filter, and pSi nanoparticles, and all materials showed maintained porous structure after the reaction with the microwave. Moreover, the coupling chemistry with diverse molecules can be added to the modified surface of pSi.

## Process Optimisation of Carbon-based Nanomaterials Production for Sustainable Energy Storage Devices: The key to Lead the Energy Transition for the 4<sup>th</sup> Industrial Revolution

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### Abstract

Carbon-based materials have received increasing attention because of their characteristics to perform as highly efficient electrode materials for supercapacitors, however, these are costly and not environmentally friendly. The production of these novel materials is limited by the lack of industrial-scale methods that can be time saving and economically feasible. This study addresses the challenges and mechanisms involved in synthesising nano-porous carbon materials for energy storage devices and the potential strategies to be manufactured under a sustainable framework on a large scale.

Supercapacitors have a wide range of operating temperatures, making them well-suited for harsh industrial conditions. The optimization of these sustainably sourced feedstocks aligned to new computational tools in an interdisciplinary approach offers a potential solution to fill the gap between laboratory and industrial-scale manufacturing of supercapacitors. Additionally, recycled feedstock could be set out as an alternative to powering the circular economy for plastics.

Energy storage systems are ubiquitous across industrial processes, from power generation to logistics and manufacturing. Consequently, even marginal improvements on the sustainability of energy storage production processes are expected to result in a substantial impact on the energy transition for the 4<sup>th</sup> industrial revolution.

The growing interest of many companies towards energy transition to sustainability makes energy storage systems sustainably manufactured the cornerstone to support this process, especially for power generation, distribution and in industry 4.0. applications.

## Single Atom Platinum-implanted 2D MoAl<sub>1-x</sub>B MBene for High-performance Hydrogen Evolution Reaction

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### Abstract

Hydrogen gas, nowadays, is emerging as a promising energy carrier source for future green and clean society and economy due to their high energy density and zero-pollution emissions. For producing high-purity hydrogen gas, the electrochemical hydrogen evolution reaction (HER) is one of the most promising technologies. Platinum group metals have been known as the state-of-the-art of electrocatalysts for facilitating HER at cathode; however, the high cost and scarcity greatly deter their practical usages. Therefore, maximizing the using amount of Pt catalysts without sacrificing high activity is urgently required so far. Two-dimensional (2D) MoAlB MBene, a member of layered ternary borides, has recently attracted much attention for catalyst development due to its excellent oxidation resistance, metallic conductivity, and hydrophilic ability. Since they have superior properties among well-known 2D materials and also possesses structure similar to graphene sheets, it is expected an outstanding substrate to disperse active catalysts, and then result in particular synergistic effects for improving catalytic performance. Herein, we construct a novel electrocatalyst based on Pt single atoms (SA) anchoring onto layered MoAl<sub>1-x</sub>B sheets. By breaking the size limitations, Pt<sub>SA</sub>-MoAl<sub>1-x</sub>B possesses a high Pt atom utilization along with abundant electroactive sites, thereby leading to highly intrinsic HER activities. In alkaline medium, the Pt<sub>SA</sub>-MoAl<sub>1-x</sub>B catalyst requires an overpotential of 30 mV to reach 10 mA cm<sup>-2</sup>, higher than pristine MoAlB and also comparable to the benchmark Pt/C. This work introduces a perspective pathway for developing potential metal SA-MoAl<sub>1-x</sub>B MBene hybrids as highly efficient electrocatalysts towards HER.

### Acknowledgement

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## Hierarchical Three-dimensional Fe Atoms-incorporated MXene/Graphene Hydrogel Networks for Efficient Overall Water-splitting

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### Abstract

For developing renewable energy sources, electrochemical water splitting is one of the most promising techniques to produce green hydrogen gas. However, hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) are still challenging due to the difficult dissociation of water molecule step and sluggish reaction. Currently, the noble metal groups are still the benchmark electrocatalysts, such as Pt(Pd)/C for HER and RuO<sub>2</sub>(IrO<sub>2</sub>) for OER. Unfortunately, the high-cost and limited-resource of noble metals have critically deterred their applications. To overcome this issue, it is imperative to develop the low-cost and earth-abundant electrocatalysts having outstanding activities and commercial visibility. Recently, two-dimensional (2D) MXenes are of great concerns for high-performance water splitting. Particularly, the formation of a hierarchical porous structure derived from MXenes and graphene (Gr) nanosheets serving as three-dimensional (3D) linker/supporter can lead to the maximum accessible active centers and high conductivity. In an effort to further improve water splitting performances, we fabricate

a novel electrocatalyst derived from atomically dispersed single-atom iron ( $\text{Fe}_{\text{SA}}$ ) incorporated 3D  $\text{Mo}_2\text{TiC}_2\text{-Gr}$  nanoarchitectures ( $\text{Fe-Mo}_2\text{TiC}_2\text{-Gr}$ ). The synergistic effects of  $\text{Fe}_{\text{SA}}$  and  $\text{Mo}_2\text{TiC}_2\text{-Gr}$  enable highly active HER and OER activities through more multiple active sites and optimized electronic structure. As a result, the electrochemical cell of the  $\text{Fe-Mo}_2\text{TiC}_2\text{-Gr}$  (+/-) reaches a current response of  $10 \text{ mA cm}^{-2}$  at a cell potential of 1.61 V, suggesting good catalytic performance of the  $\text{Fe-Mo}_2\text{TiC}_2\text{-Gr}$  for HER, OER, and then overall water splitting.

### Acknowledgement

This research supported by The Regional Leading Research Center Program (2019R1A5A8080326), Basic Science Research Program (2020R1F1A1075921) and BRL Program (2020R1A4A1018259) through the National Research Foundation (NRF) funded by the Ministry of Science and ICT, Republic of Korea.

## Controlling the Structure of Metal and Polymer Foams via Advanced Templating Approaches

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### Abstract

Inertial confinement fusion (ICF) experiments can access the extremely high temperatures and pressures required to initiate and observe nuclear fusion reactions and allow material properties to be studied at high energy densities. Accordingly, ICF targets have stringent material properties, requiring versatile fabrication methods which can synthesise microporous metal and polymer foams with highly tunable, bespoke material properties, whilst also providing reproducible control of density, uniformity, and void sizes. Current strategies employ templating methods involving commercially manufactured polymer microspheres, however, polymer microbead templates generated using microfluidics may offer considerable advantages in flexibility and precision. With this in mind, the primary aim of this work is the development of a novel fabrication method for metal foams which employs polymer microbeads, synthesised using droplet microfluidics, as templates that are explicitly designed to influence the properties of the final material.

A microfluidic platform capable of generating polyacrylate microbeads with uniform size distributions of 150 - 190  $\mu\text{m}$  has been developed, utilising glass capillary-based microfluidic devices, with size control of microbeads demonstrated by variation of microfluidic flow parameters. Following this, as a proof of concept, copper foams templated using polyacrylate microbeads synthesised without the use of microfluidics were fabricated and characterised by XPS, TGA, and SEM. Results show that polyacrylate microbeads could make suitable templates for copper foams, and that a similar concept can also be applied to the templating of pure polystyrene foams.

## Functional Properties of Transparent Epoxy-based Nanocomposite Coatings

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### Abstract

The goal of the work was to improve hydrophobic properties of transparent epoxy-based coatings. The research involved the use nanosilica particles for modification of coatings roughness. For this purpose, three methods of nanosilica

deagglomeration was utilized: magnetic stirring, ultrasonication and calendaring. Influence of chemical composition modification on physical and functional properties of investigated coatings was examined. Viscosity and gel time were determined to assess the effect of nanosilica content on processing properties. To verify wettability behaviour, water contact angle, contact angle hysteresis and sliding angle were measured. Moreover, surface topography and roughness was measured using light profilometry. Transmittance and reflectance were also measured to assess how performed modification influenced optical properties. Obtained results showed that addition of nanosilica increases hydrophobic properties of transparent epoxy-based coatings without deterioration of their optical properties.

## Effect of Chemical Modification of Transparent Silicone-epoxy Coatings on Their Hydrophobic Properties

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### Abstract

Over the last years, transparent coatings have become very popular due to their variety of applications. Such coatings are used on the surfaces of photovoltaic modules, glass skyscrapers, or aircraft, among others. These coatings are exposed to external factors, which include dust, dirt, snow, ice, or UV radiation. Given this, coatings must meet appropriate requirements, which, in addition to high durability, include having self-cleaning and ice-phobic properties. These properties can be achieved by improving the hydrophobicity of the surface. The solution is based on the idea that a highly hydrophobic material can spontaneously remove accumulated contaminants along with water droplets, while at negative temperatures it maximally reduces the contact time of the cooled droplets with the surface and, as a result, prevents the formation of ice (or frost) and reduces its adhesion. In the present study, the epoxy-silicone hybrid resin was modified with organosilicon modifiers. These compounds provide high compatibility and reactivity with the polymer matrix and can be functionalized with low-polarity functional groups that direct the properties to be hydro- and ice-phobic. The work presents preliminary results on viscosity, gel time, wettability (water contact angle, contact angle hysteresis, roll-off angle), roughness, and transmittance of modified epoxy-silicone coatings.

## Influence of Dry Etching Plasma Treatment Energy on the Tensile Strength and Surface Appearance of Bamboo Fibers

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### Abstract

Nowadays, the use of natural fibers in composite industry have been increased. Nevertheless, its uses are limited due to the incompatibility with common matrices, mainly polymeric matrices. This limitation can be overcome treating fibers using physical or chemical procedures. The main purpose of physical procedures is to change the fiber's structural and surface properties; these modifications can be achieved through plasma, vacuum ultraviolet irradiation, ozone, corona, and laser treatments, among others.

Plasma treatments fulfill three main purposes: surface functionalization, thin film deposition, and etching. In dry etching, the material is removed from the fiber surface (using purely physical processes, which can be achieved by physical sputtering procedure, in which the material is removed) through the ion bombardment induced by the plasma.

This work shows the results obtained in research aimed to study the influence of dry etching plasma treatments with different energies on the tensile strength and surface appearance of bamboo fibers. Results show that the plasma ion bombardment affect the appearance of the surfaces and change the tensile strength. On the other side, the effects produced both in the surface morphology and tensile strength of the bamboo fibers by changing the plasma energy do not be appreciable, but the same results can be achieved with less bombardment time.

## Designing and Testing New Peptide-based Molecules for Biotechnological Applications

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### Abstract

Recently, a new system of 2D cell culture was developed to produce adherent cells at quantities relevant for industrial-scale applications. This system utilises a bioreactor designed to enable the continuous culture of adherent cells, and a smart peptide surface coating that promotes cell attachment, growth, and allows self-detachment of cells at the single cell scale through cleavage of the peptide by endogenously expressed enzymes. However, cellular enzyme expression levels can vary, resulting in self-detachment at different rates, and potentially leading to lengthy optimisation phases for achieving equilibrium between cell detachment and cell replacement rates via proliferation.

Therefore, a new smart coating has been developed comprised of peptide amphiphiles (PA), synthetic peptides capable of self-assembly into nanostructures. This PA has also been designed to promote cell attachment and growth but includes a cleavable sequence that will facilitate single-cell detachment with the addition of a commercially viable enzyme. This will enable collection of detached cells for further downstream applications, and the proliferation of still attached cells will repopulate the culture. Finally, the design of this system allows it to be readily compatible with any cell type.

So far, the PA is observed to self-assemble into highly organised nanofibres comprised mainly of beta-sheet secondary structures. The PA is also capable of forming uniform surface coatings, and incubation with the cleavage enzyme indicates successful cleavage. Currently, coated surfaces are being cultured with C2C12 cells which will be assessed for successful attachment, their rate of proliferation and migration, and capacity for detachment and reattachment.

## Dual-atomic Pd and Ru-Implanted MoS<sub>2</sub> Nanosheets for Synergistically Accelerating Solar-assisted Alkaline Water Electrolysis

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### Abstract

For large-scale production of green hydrogen fuel via water splitting, the development of cost-effective and high-performance electrocatalyst is necessary. The noble metal-based nanomaterials, such as Pt/C and RuO<sub>2</sub> (IrO<sub>2</sub>) have been considered to be the state-of-the-art electrocatalysts to effectively promote cathodic hydrogen evolution reaction (HER) and anodic oxygen evolution reaction (OER), respectively. However, the high cost, scarcity, and inadequate stability are the critical limits for their extensive applications. To address this issue, recent efforts have focused on the rational design of single atom (SA) catalysts as a promising alternative for future catalyst industry. Herein, we study on a novel electrocatalyst derived from the dispersion of dual-atomic Pd and Ru via metal-S coordination in two-dimensional MoS<sub>2</sub> nanosheets coating over high-conductive CoNi alloy nanowires (CoNi@MoS<sub>2</sub>-Pd<sub>SA</sub>Ru<sub>SA</sub>). The achieved CoNi@MoS<sub>2</sub>-Pd<sub>SA</sub>Ru<sub>SA</sub> material can obtain tailored properties to impressively

improve both of the HER and OER in alkaline medium. The CoNi@MoS<sub>2</sub>-Pd<sub>SA</sub>Ru<sub>SA</sub> shows HER and OER overpotentials as low as 89 and 230 mV at a current response of 10 mA cm<sup>-2</sup> in alkaline freshwater, respectively, along with good stability. The electrolyzer of CoNi@MoS<sub>2</sub>-Pd<sub>SA</sub>Ru<sub>SA</sub>(+,-) delivers small cell voltage of 1.45 at 10 mA cm<sup>-2</sup> and high solar-to-hydrogen conversion efficiency of 17.7% in freshwater, surpassing the performances of Pt/C<sub>(-)</sub>//RuO<sub>2(+)</sub>-based device. The results open a potential approach to fabricate high-efficiency electrocatalyst for producing green hydrogen fuel via electrochemical water splitting.

### Acknowledgement

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## Origin of Particle Defects on Cleaned GaSb Substrate

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### Abstract

Gallium antimonide (GaSb) is becoming increasingly important as the substrate for applications in infrared detectors, infrared LEDs and lasers and transistors due to the parameter matching of various ternary and quaternary III-V compounds. With the device dimensions continuing to shrink and particle identification techniques and removal processes both becoming less effective due to the decreasing particle size, the identification and removal of particle defects from GaSb wafer surfaces are becoming an increasingly challenging problem. In the present study, statistical analysis of a large number of particles from multiple perspective were performed using a variety of experimental methods. The objective of the study is to master the law of particles adsorption on surface and propose effective ways for process improvement by analyzing the composition and source of residual particles on GaSb surface.

It can be found that residual particles, which composed by metal and non-metal ions, can be roughly divided into five categories based on the composition. From TOF-SIMS results, the non-metal ions that make up particles are uniformly distributed, while the metal ions are very unevenly distributed. In addition, with the continuous increase of the exfoliation sputtering depth on the surface of the GaSb substrate, only Ga and Sb elements are detected as elements, which indicates that the impurity particles are the result of adsorption during wafer processing. In this work, we analyze the source and formation mechanism of the particles in detail according to the composition of the residual particles on the surface of the GaSb substrate.

## Synthesis and Characteristics of ZnGa<sub>2</sub>O<sub>4</sub> Polycrystalline Films by Sol-Gel Method Using Rapid Heating

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### Abstract

Spinel-type oxide ZnGa<sub>2</sub>O<sub>4</sub> (ZGO) is a thermally and chemically stable semiconductor with a large energy gap above 4.8 eV. Therefore, it is expected to be applied to optoelectronic devices. In this study, polycrystalline thin films of ZGO were synthesized on the surface of synthetic quartz substrates by a sol-gel method using rapid heating, and the structural and optical properties specific to the synthesis method were investigated. The substrate was spin-coated with a precursor gel, inserted into a heated electric furnace, held for 10 minutes, and then withdrawn. The

sample was prepared by repeating this process five times. The heat treatment temperature was varied from 300 to 900 °C. The products on the substrate surface after heating were evaluated by XRD, SEM, EDX, and PL. As a result, the formation of ZGO polycrystalline films were confirmed in the samples heat-treated at 600 °C or higher. The crystallite size increased with increasing temperature, and a broad peak in the green region around 500 nm and a sharp peak in the red region around 700 nm were observed in the PL spectrum. These results indicate the possibility of individually controlling the emission intensity at different wavelengths in ZGO polycrystalline films in a short time without doping other elements.

## Effect of Growth Conditions on Luminescence Properties of CVD Nanodiamonds with SiV and GeV Color Centers

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### Abstract

Nanodiamonds with embedded luminescent color centers, being biocompatible non-toxic materials that demonstrate bright and photostable emission, are considered promising fluorescence labels for bioimaging. The surface of nanodiamonds can be chemically modified for biological targeting. Nanodiamonds with color centers based on group IV elements, such as the negatively charged silicon vacancy (SiV<sup>-</sup>) and germanium vacancy (GeV<sup>-</sup>) are attracting much interest owing to the narrow zero-phonon line, weak electron-phonon coupling, and short photoluminescence lifetime. The nanodiamonds with simultaneously embedded luminescent GeV<sup>-</sup> and SiV<sup>-</sup> color centers from solid sources were produced by the hot filament chemical vapor deposition technique (HFCVD) under different growth conditions. The nanodiamonds spectra show narrow zero-phonon lines at 602 and 738 nm of GeV<sup>-</sup> and SiV<sup>-</sup> color centers, respectively, whose intensities strongly depend on the growth conditions. It was found, that the absolute and relative intensity of zero-phonon lines of the GeV<sup>-</sup> and SiV<sup>-</sup> centers strongly depend on the methane concentration in the mixture, the substrate temperature, and the growth time. The optimal CVD growth parameters (substrate temperature of 630–700 °C and methane concentration of 4–5%) were established which corresponds to the fabrication of nanodiamonds with comparable zero-phonon line intensities of the GeV<sup>-</sup> and SiV<sup>-</sup> centers. The obtained result makes it possible to tune the growth parameters of HFCVD to redistribute the intensities of luminescent responses of color centers embedded in nanodiamonds for tailoring bicolor fluorescence nanodiamond labels.

### Acknowledgement

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## The Effect of Silanized Bentonite on Rheological Behavior of Polymer Blends

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### Abstract

The rheological behavior of filled polymer blends is an ever-expanding field in the polymer industry today. Recently, many studies have been focused on the rheological behavior of filled polymer materials, where the filler affects not only material exploitation characteristics, but essentially determines its fabrication into a final product. The behavior of polymer materials reinforced with fillers need to be understood deeply to clarify the rubber-filler interaction and its effect on rheological behavior of filled rubber blends. Furthermore, using silane, the studies were conducted to achieve better filler dispersion and rubber-filler interaction. The RPA stands for a rotational shear rheometer

dedicated to the viscoelastic characterization of polymer materials and rubber blends at all stages of manufacturing. The work was focused on the investigation of silanized bentonite effect on rheological behavior of polymer blends. The two types of silanized bentonites were added into polymer blends as a partial replacement of the commonly used filler – carbon black. In this work, a rubber process analyzer (RPA) was used to determine the changes in the curing characteristics as well as filler-filler and filler-polymer interactions by the Payne Effect before and after crosslink formation. This research work has been supported by the Operational Program Integrated Infrastructure, co-financed by the European Regional Development Fund by the project: Advancement and support of R&D for “Centre for diagnostics and quality testing of materials” in the domains of the RIS3 SK specialization, Acronym: CEDITEK II., ITMS2014+ code 313011W442.

## Effect of Different Types of Plasticizers on the Properties of Elastomeric Blends Filled with Biopolymer

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### Abstract

The oil derivatives plasticizers are commonly used to achieve better processing and the desired properties of elastomeric blends. Plasticisers based on oil derivatives have a negative impact on the environment due to their production and application. For the above reasons, research has been focused on finding the alternatives of conventional plasticisers, namely from renewable sources. The aim of the study was to determine the impact of sustainable plasticizers on the properties of elastomeric blends based on natural rubber (NR) filled with cellulose (CEL). The effect of low-content polycyclic aromatic hydrocarbon plasticizers – RAE (residual aromatic extracts) and MES (slightly extracted solvate) compared with natural oil plasticizers – linseed oil (LO), rapeseed oil (RO) was investigated. Vulcanisation characteristics, rheological and physical–mechanical properties were studied for prepared NR/CEL blends with different types of plasticisers. Based on the obtained results, NR/CEL blends with linseed oil showed comparable values to the conventional plasticisers. In the case of blends filled with bio-fillers, it is possible to eliminate an ingredient based on petroleum products in order to preserve the possibility of biodegradation. This research work has been supported by the Operational Program Integrated Infrastructure, co-financed by the European Regional Development Fund by the project: Advancement and support of R&D for “Center for diagnostics and quality testing of materials” in the domains of the RIS3 SK specialization, Acronym: CEDITEK II., ITMS2014 + code 313011W442.

## Influence of Filler on Structural and Surface Properties of Elastomeric Composites

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### Abstract

Characterization of elastomer composite morphology, mainly phase morphology, cure state variations, polymer-filler interactions and filler phase distribution are critical in establishing the morphology-property relationships for composites consisting of elastomeric composites. This work deals with preparation of elastomeric composites filled with biopolymer. Natural rubber (NR) was filled with cellulose (CEL) in amounts 30 – 55 phr. Filler/plasticizer partition in elastomeric composites, compatibility and interfacial adhesions between matrix and filler can be measured. Applications of quantitative AFM morphological analysis to design better elastomer composites are presented. Dynamic mechanical properties of NR/CEL composites were measured in the temperature range from –30 °C to 100 °C. The properties were compared with those from materials of the same composition but without filler (CEL). The laboratory tests show differences in Elastic modulus ( $E'$ ), Loss modulus ( $E''$ ) and glass transition temperature

changes in Tan Delta observations ( $\tan \delta_{max}$ ). This research work has been supported by the Operational Program Integrated Infrastructure, co-financed by the European Regional Development Fund by the project: Advancement and support of R&D for “Center for diagnostics and quality testing of materials” in the domains of the RIS3 SK specialization, Acronym: CEDITEK II., ITMS2014 + code 313011W442.

## Electroconductive Coatings Based on Poly(L-DOPA)-functionalized Graphene

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### Abstract

Graphene due to its excellent thermal, electrical, mechanical, and optical properties is still becoming a very popular candidate to be used in electronics, materials engineering, and medicine. However, fully exploiting of the graphene's potential is rather problematic since graphene exhibits strong van der Waals inter-flake interactions and hence being hydrophobic tends to disperse in nonpolar solvents. On the other hand, in the production processes one prefers using nonvolatile, nontoxic, and eco-friendly solvents e.g. water. This entails many difficulties related to the compatibilization of graphene with matrices and hydrophilic liquids.

Herein, we present the mussel-inspired functionalization of graphene with polylevodopa (PDOPA). Based on thermogravimetric analysis (TGA) and transmission electron microscopy (TEM) we found that the polymerization of L-3,4-dihydroxyphenylalanine (L-DOPA) led to decoration of graphene flakes with 10-20 nm PDOPA layers (23 wt.%). We have also demonstrated that PDOPA-coated graphene forms a homogeneous and long-time stable dispersion, which enable the production of low resistivity coatings ( $1.9 \text{ k}\Omega \text{ sq}^{-1}$ ). The measurement of the rheological properties of the paints confirms that high viscosity at low shear rates ( $0.4 \text{ Pa}\cdot\text{s}$  at  $20 \text{ s}^{-1}$ ) helps maintain product consistency for a long time, what makes it a very promising material to be used in textronics, radar-absorbing materials, or electromagnetic interference shielding.

## Colloidal Synthesis of NaSbS<sub>2</sub> Based Mixed Ionic-electronic Conductor: The Role of Temperature, Ligand and Precursor

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### Abstract

Mixed ionic and electronic conductors (MIECs) have been explored for long, due to their favorable properties for energy storage application. However, many technological relevant mixed ionic and electronic conductors contain toxic, heavily regulated (Pb) or relatively scarce elements (Li) with high manufacturing cost. Here, we report

a low temperature, shape and size tunable (50 – 90 nm) colloidal hot injection approach using widely available precursors for synthesizing sodium-antimony chalcogenide nanocrystals based on earth abundant and non-toxic elements. Three synthetic parameters, reaction temperature/, cationic precursor/, and added ligands are explored as a handle to control the size and shape of NaSbS<sub>2</sub> nanocrystals with the impact on nucleation and/or growth of NCs. Surface chemistry reveals carboxylate and related ligands are passivated to the surface of ternary nanocrystal. The electronic ( $3.31 \times 10^{-10}$  S cm<sup>-1</sup> (e<sup>-</sup>) and ionic ( $1.9 \times 10^{-5}$  S cm<sup>-1</sup>) conductivities of the synthesized NaSbS<sub>2</sub> NCs have been experimentally demonstrated using impedance and DC polarization techniques. Overall, this synthesis provides mechanistic insight and post synthetic evaluation of factors controlling the synthesis of alkali metal based chalcogenides materials behaving as MIECs.

## Formation of Quaternary and Pentanary CuZnGeS<sub>4</sub> (CZGS) Nanorods and 1-D CuZn-SnGeS<sub>4</sub> (CZTGS) and Using Colloidal Routes with In-situ Partial Cation-exchange Mechanism

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### Abstract

Cu<sub>2</sub>ZnSnS<sub>4</sub> (CZTS) nanocrystals have potential application in the photovoltaics field due to earth-abundant elements and high absorptivity. However, to achieve efficiencies as high as those reported for Cu(In,Ga)S<sub>4</sub>-based devices, the performance of these solar cells must be improved. In this regard, the controlled addition of Ge in CZTS allows an increase in the band gap towards the optimum value of 1.5 eV since the band gap of CZTS is dropped to 1.1 eV during the selenization process in photovoltaics device. Herein, we first-time report the synthesis of 1-D CZTGS nanorods (NRs) with incorporation of 'Ge' into the quaternary CZTS NRs via in-situ partial cation exchange using hot-injection method. Arrow-shaped 1-D NRs CZTGS formed by in-situ partial-cation exchange of Sn molecules from Ge molecules into the CZTS system showed polytypism between zinc-blende and wurtzite phase. Additionally, we optimized the Ge-concentration to better replace Sn in the unit-cell of the CZTS nanocrystal. We further synthesized the orthorhombic CZGS NRs by following the same protocol as CZTGS without 'Sn'. We identified the critical control parameters in this system and showed that the solvents, surfactants, ligands and precursors used are essential. Additionally, the formation-mechanism of CZTGS and CZGS NRs was observed by aliquots study as the chemistry of Ge precursor dissolution in low-temperature operations was not well-explored. Furthermore, we studied the optical properties of CZGS and CZTGS using UV-VIS and compared them with cyclic-voltammetry data, which showed promising results for further applications.

## First-principles Study of Structural, Elastic, Mechanical and Electronic Properties of Martensitic Transformation of FeX (X=Pd, Pt)

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### Abstract

The structural elastic and electronic properties of the FeX (X = Pd, Pt) are investigated by *ab initio* simulation using a pseudopotential approach within the density functional theory (DFT) method. As our exchange functionals we have considered both the generalized gradient approximation with dispersion correction (GGA + WC) and the local density approximation (LDA), respectively. The crystal structure of FeX (X = Pd, Pt) is described and compared

with other similar compounds. This structure crystallizes in the rock-salt (phase A1, NaCl, 225) space group Fm-3m in the austenitic phase and in FCT (face centered tetragonal) (P4 / mmm, L1<sub>0</sub>, N ° 123) space group P4/mmm in the martensitic phase. The enthalpy of formation of the martensitic phase of the compound FePd [FePt] is -3328 eV [-3168 eV], is -6645 eV [-6326 eV] of the austenitic phases. The martensitic phase is stable by tetragonal distortion and the martensite of FePd is more stable. The bulk modulus along the crystallographic axes of single crystals is calculated using the GGA + WC. The martensitic compounds FeX (X = Pd, Pt) is an anisotropic material. We only focus on the important contributions of the elements Fe: 3d-4s, Pd: 4d-5s and Pt: 5d-6s, we show the calculated partial densities of these states of the 2FeX (X = Pd, Pt) martensitic structures respectively. Our results for the equilibrium lattice constants are in good agreement with the experimental data.

## Improving the Superconducting Characteristics of Single-Crystal FeTeSe by Hydration Method

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### Abstract

The electronic, current-carrying, and magnetic characteristics of perspective high-temperature superconductors (HTSC) based on iron-chalcogenides are very sensitive to various doping. For a wide number of compounds, including metallic, cuprate, pnictide- and FeSe-based materials, an impact of hydrogen causes a perceptible improvement in their superconducting properties.

To increase the current-carrying capacity of FeTe<sub>0.65</sub>Se<sub>0.35</sub>, studies were made of the effect of hydrogen gas sorption on the structure for this type of HTSC single-crystal compound, on the maximum achievable current densities, on the effective pinning potential of trapped magnetic fluxes, and on the effect of a constant magnetic field.

The experimental FeTe<sub>0.65</sub>Se<sub>0.35</sub> single crystals were grown from the melt by the Bridgman method. Hydration by method of hydrogen gas sorption was performed at several values of temperature, pressure, and time of the samples processing. The temperature of the samples during this procedure varied from room temperature (20 °C) to 250 °C, and the pressure from 10<sup>-6</sup> to 5 atm. The time of interaction of gaseous hydrogen at room temperature in some experiments reached 720 h.

It has been found that the mechanisms of hydrogen sorption and the crystal symmetry change with an increase in the sample temperature. Under the influence of the catalytic action of Fe atoms in FeTe<sub>0.65</sub>Se<sub>0.35</sub> + H<sub>2</sub> solutions at a temperature of about 200 °C, dissociation of hydrogen molecules occurs. This process is accompanied by an increase in the value of mechanical stresses, as well as inhomogeneity of local deformations of interatomic chemical bonds.

It was shown that hydrogenation strongly affects superconducting properties of FeTe<sub>0.65</sub>Se<sub>0.35</sub> single crystals. Bulk critical temperature increases by 1–2 K and transition to superconducting state becomes sharper. The new effective pinning centers are appeared and obtained high values of the thermal activation energy U were 0.5 eV < U < 1.0 eV. Determined in magnetic field range of 0–70 kOe the critical current density increases up to ~ 30 times compared with pristine sample as a result of hydrogenation at 200 °C for 10 h at gas hydrogen pressure of 5×10<sup>5</sup> Pa.

## Manufacture and Characterization of Benzoxazine Resin with 5% v/v açai Biomass Composites

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## Abstract

Agroindustry residues, once unusable, have been re-entered into the production cycle, either by imposing environmental laws aimed at reducing their disposal in landfills, by reducing manufacturing and consumption costs of petroleum derivatives or by their physical-chemicals characteristics that interesting properties to the final pieces. Within this scenario, composites using natural fibers have been standing out. In Brazil, the biomass from the exploitation of açai fruits has gained visibility since the large amount of waste from this process is underused. In the case of matrices, benzoxazine resin has been standing out for being a high-performance polymer, with high temperature resistance, low moisture absorption and which does not generate by-products during its curing. Therefore, composites were made using benzoxazine resin and 5% v/v of açai biomass in natura and hydrothermally treated (121 °C for 45 minutes, 1.05 bar) and cured in a conventional oven (RT up to 190 °C - 7 days). The thermal characterizations of the cured composites, via thermogravimetry, demonstrate that the degradation temperatures did not undergo considerable changes when compared to the pure resin. The glass transition values, obtained in DSC, show an increase with the addition of biomass, a fact confirmed by the DMA tests. Therefore, the use of this biomass in the composite reduces the amount of polymer matrix to be used, contributes to the environment through recycling, expanded the range of applicability in relation to the working temperature of the material and may reduce the cost of the final part.

## A Comparative Spectroscopic Study of Polyvinyl Alcohol and Pectin Films Loaded with Silver Nanostructures with Different Sizes and Shapes with Tuneable Plasmonic and Electric Properties

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## Abstract

Electrochemical Impedance Spectroscopy (EIS) was used to study the electrical behavior of polymer nanocomposite films prepared by embedding silver nanostructures (AgNPs) in different polymeric matrices, namely polyvinyl alcohol (PVA) and pectin (PEC). The results indicate that the conductivity of the PVA is increased by incorporating AgNPs, and it is highly dependent on the size and shape of the AgNPs embedded into the polymer, where a steady decrease of the impedance was observed for smaller AgNPs in a PVA matrix. Nanocomposites films from PVA also involved a pronounced hypsochromic shift of the surface plasmon resonance band as the silver nanostructures are incorporated into the polymer matrix. On the other hand, a very different behavior was obtained for nanocomposites films consisting of AgNPs embedded in a PEC matrix. Once AgNPs were embedded in the PEC matrix, a decrease of the impedance of nanocomposite films was evidenced. An increasing impedance was found with increasing AgNPs size until a maximum is reached. Regarding the surface plasmon resonance band for the system AgNPs - PEC, no evidence of shift was observed.

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