

## 4<sup>th</sup> International Conference on Materials Science & Nanotechnology (Spain 2023)

### Keynote Session

#### Graphene for Molecular Electronics

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#### Abstract

Molecular electronics offers an elegant tool to miniaturize electronic devices, reaching the nanoscale or even the single-molecule level. One of the limitations of this approach concerns the insulating character of most of the molecular systems one wants to integrate in the device. Here we show that the deposition of these functional molecules over graphene and other 2D semiconducting materials can provide an efficient way to avoid this limitation. This concept provides an entire new class of molecular/2D heterostructures in which we take advantage of using the “all surface” 2D material to sense the properties of the molecular component electrically or optically *via* an active control of the hybrid interface. We will illustrate this concept by choosing as molecular component spin-crossover molecules. This type of magnetic molecules provides an appealing example of molecular bistability as they can switch between two spin states upon the application of an external stimulus (temperature, light, or pressure) [1]. This spin switching can occur near room temperature and is always accompanied by a significant change of volume (by ca. 10%), so it can generate a significant strain over the 2D material. Hence, they constitute an ideal component to fabricate molecular memory devices. In this talk we show that in these heterostructures the 2D material can act as a reliable and highly sensitive spin state sensor, using the changes observed in the electrical or optical properties of the 2D material to readout the spin state [2-4].

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## Peripheral and Central Nerve Repair: Understanding the Clinical Problem and Strategies for Improved Outcomes

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### Abstract

Peripheral and central nervous system injuries can be traumatic for the patient, debilitating and with lifetime care required for both the patient and quite often by the families at extremely high cost to health care providers. Current solutions are suboptimal and also have significantly different requirements depending on whether the nerve damage is peripheral or central. Much interest has focused on the use of soft materials, such as hydrogels, but our research has taken a different path, informed by promising results from *in vitro* and *in vivo* experiments. We have shown that neurite regeneration requires physical cues to direct regrowth in an axial direction and have developed implant devices that provide the required physical cues. This work is currently moving towards early-stage clinical trials. Future work will see the utilisation of growth factors and cells for further enhancement of patient recovery and clinical outcomes.

## Advances in Kinetics Processes of Halide Perovskite Solar Cells for Memory, Neuro-morphic, and Optoelectronic Applications

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### Abstract

The dynamic response of metal halide perovskite devices shows a variety of physical responses that need to be understood and classified for enhancing the performance and stability and for identifying physical behaviours that may lead to developing new applications. We present a physical model in terms of delayed recombination current that explains the evolution of impedance spectra and the evolution of hysteresis in current-voltage curves. A multitude of chemical, biological, and material systems present an inductive behavior that is not electromagnetic in origin. Here, it is termed a chemical inductor. We show that the structure of the chemical inductor consists of a two-dimensional system that couples a fast conduction mode and a slowing down element. Therefore, it is generally defined in dynamical terms rather than by a specific physicochemical mechanism. The impedance spectra announce the type of hysteresis, either regular for capacitive response or inverted hysteresis for inductive response. We apply the insights in kinetics processes to the development of memristors and neurons. We address the characterization of electron diffusion and radiative emission in halide perovskites using a range of light stimulated techniques as IMPS, IMVS, and voltage controlled light emission technique (LEVS).

## 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 low dimensional materials designed for energy and environmental applications, crystallography and distribution of the atomic species are of utmost importance in order to determine their physical and chemical properties that will improve their performance, including efficiency and selectivity towards certain reactions.

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 performance.

## Chemical Tailoring of Graphene Materials for Water Remediation, Sensing, and Carbocatalysis

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### Abstract

Graphene and 2D materials are gaining increasing interest as multifunctional platforms for realizing devices and technologies for energy, sensing, biomedical and environmental applications. Key features such as high surface area, chemical tuneability and processability determines their recognition, transduction, and transport properties. Among the others, graphene oxide (GO) is particularly suitable for property-specific tailoring through many site-specific chemical manipulations of the oxygen containing functional groups at the nanosheets surface.

In this talk, I will present selected case-studies of chemically modified GO, realized at ISOF, and their applications as active materials for water purification, electrochemical sensors and carbocatalysis. I will describe our recent results on covalent functionalization procedures and design strategies for i) enhanced adsorption of emerging contaminants (i.e., per- and polyfluoroalkyl substances (PFAS), antibiotics) from drinking water, ii) electrochemical transduction for pesticides monitoring in water and ii) CO<sub>2</sub> capture and utilization in chemical transformations.

Finally, polymer-graphene based composites for water filters will be presented, with the ongoing technology transfer and validation from lab scale to industrial production.

## Self-healing Soft Robotics Using Reprocessable Polymer Networks

Guy Van Assche<sup>1\*</sup>, Seppe Terryn<sup>2</sup>, Joost Brancart<sup>1</sup>, Jessica Mangialetto<sup>1</sup>, Aleix Costa Cornellà<sup>1</sup>, Francesca Furia<sup>1</sup>, Seyedreza Kashaf Tabrizian<sup>1</sup> and Bram Vanderborght<sup>2</sup>

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### Abstract

Reversible polymer networks are covalently crosslinked polymer networks that contain bonds that are thermally reversible. This implies that at sufficiently high temperatures, which could be as low as 100 °C, the networks are sufficiently unbound to return to a liquid state, and this in a reversible fashion. This offers important opportunities for improving the sustainability of polymer networks, as it makes these materials self-healing and reprocessable at fairly low temperatures, in contrast to their irreversibly chemically crosslinked counterparts, classic elastomers and thermosets. Although self-healing, involving the rebinding of broken reversible bonds across crack interfaces, is usually considered to require chain segment mobility, we proved that it also occurs at crack interfaces in glassy thermosets.

Through a judicious combination of building blocks and a thorough insight in the fundamentals of underlying the structure-processing-property relations, we developed room temperature self-healing reversible polymer networks, including versions that are largely biobased, that can be compounded, extruded into filaments or pelletized, 3D

printed or injection-molded, reprocessed, chemically or mechanically recycled. The applicability of these materials is demonstrated in actuators, heaters, and sensors for self-healing soft robotics.

## Graphene Coatings for Remarkable Corrosion Resistance: Challenges and Circumvention

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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 ~\$250 billion to annual loss in the USA). Despite 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., like seawater). In contrast, other reports suggest the graphene coating to 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. Based on the findings, the author's group has succeeded in demonstration of durable corrosion resistance as result of development of suitable graphene coating. The presentation also assesses the challenges in developing corrosion resistant graphene coating on most common engineering alloys, such as mild steel, and include results demonstrating circumvention of these challenges.

## Materials at the Nanoscale and Beyond

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### Abstract

Molecular science has been developed to disclose the material structures and properties at the molecular level. However, aggregates, which served as the particularly useful form of materials, sometimes behave differently from individual molecules, and show annihilated or new properties. Some unique properties such as aggregation-induced emission (AIE), crystallization-induced emission (CIE), room temperature phosphorescence (RTP), aggregation-induced delayed fluorescence (AIDF), aggregation-induced anti-Kasha transition (AKT), clusterization-triggered emission (CTE), through-space interaction (TSI), mechanoluminescence (ML), aggregation-induced circularly polarized luminescence (CPL), aggregation-induced generation of reactive oxygen species (AIG-ROS), photothermal/photoacoustic (PT/PA), solid-state molecular motion (SSMM) are only identified at the nanoscale and beyond, indicating their exotic features. By virtue of the flourishing research on aggregation-induced emission, the concept of aggregate science is put forward to fill the gaps between molecules and aggregates. The established structure-property relationship of aggregates is expected to contribute to new materials and technological development. Ultimately, the aggregate science may become interdisciplinary research and serves as a general platform for academic research.

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## Chameleon Nanocarriers for Delivery of RNA Nanomedicines

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### Abstract

By early 2023, 24 gene therapy drugs and 21 RNA therapies reached the medical market. Targeted intracellular delivery remains the key requirement. For refinements of RNA nanocarriers we focus on a bioinspired, sequence-defined process including (i) Use of artificial amino acids, (ii) Precise assembly into sequences ('xenopeptides') by solid phase-assisted synthesis, and (iii) Screening for delivery and selection of top candidates. A recent chemical evolution process combined aminoethylene amino acids as polar protonatable units with novel lipo amino fatty acids (LAFs) as hydrophobic protonatable motifs. These novel double pH-responsive nucleic acid carriers utilize intracellular delivery mechanisms of both cationic lipids and cationic polymers. The endosomal pH-dependent tunable polarity of LAF was successfully implemented by a central tertiary amine, which disrupts the hydrophobic character once protonated, resulting in drastic pH-dependent change in the logarithmic (octanol/water) distribution logD from around +1 (pH 7.4) to -1 (pH 5.5). This "molecular chameleon character" turned out to be highly advantageous for pDNA, siRNA, mRNA or CRISPER/Cas9 sgRNA delivery. Noteworthy, the efficiency of best performers was up to several 100-fold higher compared to previous carriers. Transfection activity of mRNA lipoplexes was maintained even in the presence of 90% serum and even at extremely low dosage of 3 picogram mRNA (~2 nanoparticles/cell), in the range of the viral potency. mRNA lipoplexes showed great *in vivo* performance in mice with high expression levels in spleen, tumor, lung, and liver upon intravenous administration of 1 µg luciferase mRNA. With this class of delivery carriers, also CRISPR Cas9 /sgRNA or siRNA can be delivered to therapeutically modulate cell functions.

## Designing the Fluid Architecture of Biomembranes

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### Abstract

Our body contains a large number of biological membranes which enclose our cells and many intracellular organelles. These membranes, which have a thickness of only 4 to 5 nanometers, are fluid and create a flexible architecture that partitions space into many separate compartments. The membranes provide robust barriers for the exchange of molecules between the different compartments but can easily remodel their shape and topology. This re-modeling



can be studied in a systematic and quantitative manner using biomimetic model systems. In this talk, recent insights from such synthetic biosystems are reviewed, integrating experimental observations and molecular dynamics simulations with the theory of membrane elasticity [1-5].

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## Symposium I: Nanotechnology and Nanomaterials Featured Presentations

### Modeling Elasticity and Plasticity with the Complex Amplitude Formulation of the Phase Field Crystal Model

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#### Abstract

In this talk I would like to review the use of complex amplitudes to model processes in which elasticity and plasticity play an important role. This formulation exploits complex amplitudes which vary slowly in space except near defects, such as dislocation and grain boundaries while at the same time containing the information to completely reconstruct the underlying crystal lattice. The slowly varying nature lends itself to efficient computational schemes that allow the study of relatively large system sizes. A review of the state of the art will be presented which will highlight the advantages of the method has over traditional phase field and phase field crystal methods as well the challenges that remain.

### Mechanical Characterization of 1D Nanostructures: Inconsistency of Results

Sergei Vlassov<sup>1\*</sup>, Dmitry Bocharov<sup>2</sup>, Boris Polyakov<sup>3</sup>, Mikk Vahtrus<sup>1</sup>, Sven Oras<sup>3</sup>, Veronika Zadin<sup>3</sup> and Andreas Kyritsakis<sup>3</sup>

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## Abstract

In this critical study, we call attention to a widespread problem related to the vast disagreement in elastic moduli values reported by different authors for nanostructures made of the same material. As a particular example, we focus on ZnO nanowires (NWs), which are among the most intensively studied nanomaterials. Since ZnO NWs possess piezoelectric effects, many applications involve mechanical deformations. Therefore, there are plenty of works dedicated to the mechanical characterization of ZnO NWs using various experimental and computational techniques. Reported values of elastic modulus vary drastically from author to author ranging from 20 to 800 GPa. Moreover, both–diameter dependent and independent – Young’s modulus values have been reported. We give a critical overview and perform a thorough analysis of the available experimental and theoretical works on the mechanical characterization of ZnO NWs to find the most significant sources of errors and to bring out the most trustable results.

## Impact on Optical and Structural Properties of InAs/GaSb Type-II Superlattices as Consequence of Modifications in the Configurations of Their Interfaces

J.J. Jiménez<sup>1,2</sup>, D. Alshahrani<sup>3</sup>, D.C.M. Kwan<sup>3</sup>, V. Srivastava<sup>3</sup>, M. Delmas<sup>3</sup>, B.L. Liang<sup>4</sup>, D.L. Huffaker<sup>4,5</sup>, M. Kesaria<sup>2</sup> and F.M. Morales<sup>1,2</sup>

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## Abstract

Interactions with the mid-wavelength infrared (MWIR) window are important to develop emitters and detectors useful in applications related to, for instance, spectroscopy, defense or sensing of pollutant gases (e.g., CO<sub>2</sub>, NO<sub>x</sub>). State-of-the-art MWIR technologies use materials like mercury-cadmium-telluride (MCT), InSb or InAsSb, but they all have drawbacks in one way or another. Type-II superlattices (T2SL) based on combinations of III-V materials (e.g. InAs/GaSb) are a rising alternative for devices like photodetectors, lasers or phototransistors. Nevertheless, the InAs/GaSb combination has a key limitation: an -0.6% InAs/GaSb lattice mismatch, which entails an increased interfacial strain that limits both material quality and device thickness. A possible solution is inserting InSb nanolayers between both materials to form InSb-like interfaces in the T2SL, so that a strain-balanced superlattice is generated thanks to the positive mismatch induced.

Interestingly, T2SLs with InSb-like interfaces exhibit better optical quality than other approaches, but also a lower quality structure. In this work, we report a comparative structural and optical study of two InAs/GaSb T2SLs, both with InSb-like interfaces, but one of them has InSb nanolayers intentionally deposited to form InSb-like interfaces. By combining transmission electron microscopy (TEM) studies with photoluminescence measurements and band heterostructures simulations, we successfully assessed the impact of InSb-like interfaces on the quality of InAs/GaSb T2SLs. This presentation focuses on explaining the results from the perspective of comparative TEM measurements, which gave information about many important features for the optimization of these superlattices: crystallinity, epitaxy, existence of strain, and analyses of interfacial atomic intermixing and segregation.

## Secondary Porosity as a Regulator of Hydrophobicity of Nanoporous Particles

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## Abstract

Molecular dynamics simulations were used to investigate the intrusion/extrusion of water into/from silica nano-objects. Usually, their hydrophobicity is controlled chemically. We have shown a new way of shifting intrusion/extrusion pressures using the topological tuning of the porous matrix. Intrusion/extrusion pressure decreases with the number of open lateral micropores connecting main channels. This effect can be exploited to produce new materials for practical applications when the hydrophobicity needs to be regulated without significantly changing the chemistry or structure of the materials. In the computer experiments with nano-objects immersed in water, we have observed several dozens of fast water expulsion events from nano-objects. Before extrusion, water is in a metastable state which can be triggered externally. We propose to use water ejection from hydrophobic porous materials as a new propulsion mechanism for nano rockets.

## Controlling the Crystallization and Hydration State of Crystalline Porous Organic Salts

Megan O'Shaughnessy<sup>1\*</sup>, Alex C. Padgham<sup>1</sup>, Rob Clowes<sup>1</sup>, Marc A. Little<sup>1</sup>, Michael C. Brand<sup>1,2</sup>, Hang Qu<sup>1</sup>, Anna G. Slater<sup>1</sup> and Andrew I. Cooper<sup>1,2</sup>

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## Abstract

Crystalline porous organic salts (CPOS) are a subclass of molecular crystals. Compared to other classes of porous crystals, CPOS are less established, even with their wide range of promising applications in areas such as proton conduction, molecular motors, and guest capture. Several issues such as the low solubility of CPOS and their building blocks limits the choice of crystallization solvents to water or polar alcohols, hindering the isolation, scale-up, and scope of the porous material. In this work, high throughput screening was used to expand the solvent scope, resulting in the identification of a new porous salt, CPOS-7, formed from tetrakis(4-sulfophenyl) methane (TSPM) and tetrakis(4-aminophenyl) methane (TAPM). CPOS-7 does not form with standard solvents for CPOS, rather a hydrated phase (Hydrate2920) previously reported is isolated. Initial attempts to translate the crystallization to batch led to challenges with loss of crystallinity and Hydrate2920 forming favorably in the presence of excess water. Using acetic acid as a dehydrating agent hindered formation of Hydrate 2920 and furthermore allowed for direct conversion to CPOS-7. To allow for direct formation of CPOS-7 in high crystallinity flow chemistry was used for the first time to circumvent the issues found in batch. CPOS-7 and Hydrate2920 were shown to have promise for water and CO<sub>2</sub> capture, with CPOS-7 having a CO<sub>2</sub> uptake of 4.3 mmol/g at 195 K, making it one of the most porous CPOS reported to date. These findings provide new techniques to allow the discovery and control over CPOS which we believe will help advanced this area.

## A New Route to Achieve VO<sub>2</sub> Nanoparticles for Thermo-chromic Applications

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## Abstract

Vanadium oxidation can originate products of numerous compositions and crystalline varieties of the same polymorph. The monoclinic dioxide VO<sub>2</sub>(M1) has received the greatest attention, since it transforms to tetragonal VO<sub>2</sub>(R) during heating at a certain transition temperature (T<sub>c</sub>), with an implicit reversible metal-to-insulator transition, which makes it the best candidate for many applications in smart windows, switching electronics, or heat storage. In an attempt to reach its more economical and environmentally friendly fabrication, this work explains a simple, fast, dry, cost-effective, safe and clean method to achieve VO<sub>2</sub> from the hot oxidation of a metallic precursor, which



is a novel and original strategy compared to others often based on  $V_2O_5$  reduction. Following an extensive design of experiments, V nanoparticles were thermally treated in air in ranges from 400 to 800 °C and different heating and cooling rates, and the products were studied by SEM, TEM, XRD, DSC, TGA, TPO, and MS. M1-VO<sub>2</sub> powders ( $T_c = 68$  °C) with better thermochromic properties than commercial ones were obtained by fast heating of 42°C/s in addition to (a) keeping 700 °C for about 10 min plus slow cooling (1 time); or (b) 625 °C for 5 min and fast cooling (2 times). The involved reactions, and the effect of tungsten addition were also studied. The effective W doping is thus demonstrated through a drop in  $T_c$  of ~20 °C but similar behaviour than the best undoped products, and mixes with lower performances (poorer in VO<sub>2</sub>) showed a  $T_c < 35$  °C ideal for smart glass if inserted in transparent matrixes.

## Metal-semiconductor-metal Heterostructures for Electrical, Optical, and Plasmonic Applications

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### Abstract

I will address the controlled formation of monolithic metal–semiconductor nanowire and nanosheet heterostructures. The main obstacles facing towards reliable synthesis of such hybrid systems are related to lateral strain relaxation, mitigating the limitations of material lattice compatibility and allow arbitrarily combined dissimilar materials unattainable in layered structures. Out of the wide range of nanowires, Ge combines a high carrier mobility, with a more than five times larger exciton Bohr radius compared to Si. Hence, Ge is of particular interest especially for the development of high speed and novel quantum devices.

The formation of axial nanowire heterostructures with atomically sharp interfaces and monocrystalline aluminum leads by using a thermally initiated exchange reaction will be presented. This enables the fabrication of an in line contacted quantum dot without requiring precise lithographic alignment of the contacts, which is one of the most challenging issues of fabricating quantum dot-based devices. Unambiguous signatures of quantum ballistic transport and electrostatically tunable negative differential resistance even at room temperature will be demonstrated and attributed to intervalley electron transfer.

Together with the wafer-scale accessibility, the proposed fabrication scheme may give rise to the development of key components for a broad spectrum of emerging Si and Ge-based devices requiring monolithic metal-semiconductor-metal heterostructures with high-quality interfaces for electrical, optical and plasmonic applications.

## Spike Propagation in a Nanolaser-based Optoelectronic Neuron

Ignacio Ortega-Piwonka<sup>1,2\*</sup>, Matěj Hejda<sup>3</sup>, Juan Alanis<sup>3</sup>, João Lourenço<sup>4</sup>, Antonio Hurtado<sup>3</sup>, José Figueiredo<sup>4</sup>, Bruno Romeira<sup>5</sup> and Julien Javaloyes<sup>1,2</sup>

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### Abstract

With the recent development of artificial intelligence and deep neural networks, alternatives to the Von Neumann architecture are in demand to run these algorithms efficiently in terms of speed, power, and component size. In this theoretical study, a neuromorphic, optoelectronic nanopillar metal-cavity consisting of a resonant tunnelling diode (RTD) and a Nanolaser diode (LD) is demonstrated as an excitable pulse generator. With the proper configuration,

the RTD behaves as an excitable system while the LD translates its electronic output into optical pulses, which can be interpreted as bits of information. The optical pulses are characterized in terms of their width, amplitude, response delay, distortion, and jitter times. Finally, two RTD-LD units are integrated via a photodetector and their feasibility to generate and propagate optical pulses is demonstrated. Given its low energy consumption per pulse and high spiking rate, this device has potential applications as building blocks in neuromorphic processors and spiking neural networks.

## Correlation Between Charge Density Wave Phase Transition and Hydrogen Adsorption in 1T-TaS<sub>2</sub> Thin Film Devices

Yasushi Ishiguro\*

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### Abstract

Thin film of tantalum disulfide in the 1T-polytype structural phase (1T-TaS<sub>2</sub>) is a type of metallic two-dimensional transition metal dichalcogenides. The 1T-TaS<sub>2</sub> undergoes a series of charge-density-wave (CDW) phase transitions. In the CDW phase transition, the phase changes from low to high temperature in the order of commensurate CDW (CCDW) phase, nearly commensurate CDW (NCCDW) phase, and incommensurate CDW (ICCDW) phase. The CCDW–NCCDW phase transition occurs at approximately 180 K, and the NCCDW–ICCDW phase transition at approximately 350 K; each transition exhibits an abrupt change in the electronic resistance with a temperature hysteresis ( $\Delta T$ ) behavior. We found that the  $\Delta T$  decreases in the NCCDW–ICCDW phase transition as the number of layers decreases. The layer-number dependence is the opposite behavior of the transition between the CCDW and NCCDW phases. The difference in the layer-number dependence is mainly explained by the difference in the CDW superstructure along out-of-plane direction between the CCDW and ICCDW phases. Regarding the effect of hydrogen (H<sub>2</sub>) adsorption on 1T-TaS<sub>2</sub> thin film devices, the metallic ICCDW phase exhibited high H<sub>2</sub> sensing performance. The electrical resistance of the ICCDW phase decreased when H<sub>2</sub> was adsorbed on the surface. In contrast, the NCCDW phase, which has slight band overlap or a small bandgap, was not reactive for H<sub>2</sub> adsorption. These results will clarify the physics of the 1T-TaS<sub>2</sub> CDW phase transitions and in the development of device applications using the CDW phase transition in 1T-TaS<sub>2</sub>.

## Graphene/TiO<sub>2</sub> as Electron Transport Layer to Enhance Energy Efficiency of Perovskite Solar Cells

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### Abstract

In the field of the energy transition, developing efficient and cost-effective solar cells is a crucial goal to establish an optimal energy mix. The third generation of photovoltaic cells, which utilize abundant materials and simple processes, has emerged to achieve this goal. Among these, photovoltaic cells based on perovskite materials have demonstrated significant advances, with power conversion efficiencies reaching up to 22%. However, efforts are still needed to improve these cells' charge generation and collection. One strategy to achieve this is using TiO<sub>2</sub>/graphene nanocomposites, which have been shown to reduce recombination phenomena and improve electron collection. The technique of laser pyrolysis is used to achieve high-quality nanocomposites with suitable properties for efficient and stable solar cells. This technique enables the synthesis of nanoparticles in a single step with a continuous flow. Tests were conducted using a MAPI-Cl perovskite deposited in a single-step, and the results show an increase in electron injection efficiency and device performance with the use of graphene in the mesoporous TiO<sub>2</sub> layer. Overall, the use of this technique resulted in an increase in power conversion efficiency from 14.1% to 15.1% for these devices, demonstrating the benefit of the laser pyrolysis process for the production of high-quality electron transport layers in perovskite solar cells.

## Unveiling Near-field Interactions of Metal Nanoparticles in Aqueous Solutions: Visualization Through Thermoelastic Optical Microscopy and X-band Microwaves Response of Structural Clusters

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### Abstract

In this study, an aqueous solution containing different metal nanoparticles (NPs) was examined using a thermoelastic optical microscope (TEOM) operating in the microwave X-band frequency range (8 - 12 GHz). The near-field interaction between the radiated microwaves and the aqueous solution with Ag, Pt, Au, Fe NPs, which were prepared through a laser ablation process, exhibited sensitivity to both the NPs concentration and their structural characteristics at the resonant frequency. The experimental evaluation of the maximum concentrations of the metal NPs ranged from 0.03 to 1.33 mg/ml. The measured minimum detectable normalized signal was found to be between 0.01 and 0.05 (mg/ml)<sup>-1</sup>. The exceptional sensitivity of the measurement system can be attributed not only to variations in the electromagnetic properties of the solution, such as complex dielectric permittivity and conductivity, due to changes in metal NPs concentration but also to additional structural changes in water clusters resulting from the NPs suspensions. Furthermore, the results revealed a linear relationship between the averaged signal intensity, which correlated with NPs concentrations, and the size of the metal NPs. Larger sizes and higher concentrations of NPs contributed to higher signal levels and frequency responses. Moreover, the TEOM characterization method allowed for the visualization of the electromagnetic field distribution around the solution with high spatial resolution, enabling the investigation of dielectric liquid environments with different types and concentrations of metal NPs. The TEOM method demonstrated its potential for monitoring high-conducting NPs concentrations in dielectric liquid environments, thus showcasing its applicability in chemical and biophysical sensing applications.

## Single-molecule Force Studies of Chemical Revolution Processes

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### Abstract

The origin of life is believed to have been chemical reactions at mineral surfaces on the early earth. Although there have been many proposals and preliminary experiments on this topic, no definitive origin has been reported yet because of a lack of nanoscopic studies. Herein, we present the first material surface observations intended to elucidate the origin of life at the molecular level. These observations were made using a combination of Raman spectroscopy and atomic force microscopy (AFM). Pyrite (FeS<sub>2</sub>) is known to be one of the most common minerals that can provide condensation and reaction surfaces for chemical evolution. However, this mineral has mostly been studied in bulk systems, and such investigations cannot fully resolve the exact mechanisms of the specific interactions that occur on this mineral. Moreover, no direct experimental evidence has been reported regarding pyrite initiating chemical evolution at the nanoscale when it is used as a reaction surface. In this study, the quantitative force analysis performed by AFM, in which the residue of a single amino acid was mounted on AFM tips, enabled us to locate the reaction sites and to study the interaction forces between the amino acid and the pyrite surface. Our Raman spectroscopy and AFM results revealed for the first time that defective areas, with the composition FeS<sub>2-x</sub>, increase the adsorption probabilities of amino acid residues in chemical reactions on the surface of pyrite.

## Photoresponsivity of Carbon Dots/Graphene Hybrids on Flexible Substrates

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### Abstract

Carbon dots (C-dots) emerged as an exciting material for a new generation of optoelectronic devices, owing to their distinctive photophysical properties, low production costs, and non-toxicity. Leveraging the good molar absorptivity of C-dots and the efficient transport properties of graphene derivatives, a flexible photodetector with spectral responsivity in the visible range was developed.

Newly designed C-dots, using both linear and branched polymers for the carbon nanoparticle surface passivation, exhibit high photo-emission efficiency, and depending upon the surface functionality display specific emission spectra covering the entire visible domain. Polymer ramification showed no significant improvement in fluorescence quantum yield but enabled the bathochromic emission shift to 520 nm.

Tuning the oxidation/doping in the graphene derivatives and their interaction with the C-dots, the photoresponsivity of the graphene/C-dots hybrids achieved a maximum of 0.25 mA/W under white light exposure with an incident power density of 40 mW/cm<sup>2</sup> and a 5 V applied bias. When the branched C-dots were combined with the hydrothermally doped graphene oxide, the photoresponsivity increased by a factor of four as compared to the linear polymer-C-dots. Responsivity reached 1.25 mA/W at the incident power density of 70 mW/cm<sup>2</sup> and bias of 5V.

The synthesized C-dots/graphene hybrids offer the promise to develop wideband, flexible, and wearable photodetectors that do not require different material systems to cover a broad spectral range of detection.

## Pt/TiO<sub>2</sub> Single Atom and Small Cluster Catalysts Exposed to Chemical Warfare Agent, Sarin

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### Abstract

The development of new catalytic nanomaterials is extremely advantageous for the design of innovative materials capable of enhanced filtration and/or decontamination of toxic chemicals. Improved reactivity, with respect to both rate of decomposition and final degradation products, is a key objective for the design of novel catalysts. To that end, a model catalyst comprised of Pt single atoms and small clusters on a TiO<sub>2</sub> particulate support has been exposed to the chemical warfare agent, Sarin, GB. The work described herein focuses on the uptake and reactivity of GB on the Pt/TiO<sub>2</sub> catalysts. Studies were conducted in a high vacuum chamber using transmission infrared spectroscopy to monitor the reaction in real time. Results such as these can be used to further catalyst design in the future.

## Defect Nanopatterning in Low Dimensional Materials: An Approach to Impart Material Functionalities

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## Abstract

Structural defects are always present in manufactured materials and affect, or sometimes even generate their physical properties. Influenced properties include catalysis, electrical and thermal conductivity tuning, thermoelectricity, enhanced ion storage, and magnetism. These properties enable the use of defective materials in various technological applications.

To date, the research and technology in defect engineering are focused on controlling defects' nature and statistical distribution. Still, it has some crucial problems, such as the limited density of defects that can be introduced into a material without compromising its stability and the interdependence of the various effects generated by defects. Here, we propose defect nanopatterning as a breakthrough to overcome the principal limitations of current methods.

We present preliminary data about the spatially controlled defect generation using stamp-assisted electrochemical treatment. We applied the process to transition metal dichalcogenide thin films, fabricating nonmetal atomic vacancies. Our approach allows us to produce a spatially controlled nanometric zone rich in defects while preserving the original properties of materials in untreated zones. The process enables us to optimise defect distribution for target applications.

## Quercetin Mediated Synthesis of Au/TiO<sub>2</sub> Nanocomposite for the Photocatalytic Degradation of Antibiotics

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## Abstract

Water pollution is one of the world global concerns. It is estimated that 842,000 people die each year from the consumption of polluted water. Among the different contaminants, the so-called of emerging concern have raised considerable attention. They are non-regulated toxic chemicals, found in low concentrations in all types of water bodies, and very resilient to conventional water treatments. Currently, no effective methods have been found to eliminate them, however, photocatalysis has arisen as one of the most suitable possible solutions. TiO<sub>2</sub> is one of the most widely used catalysts, unfortunately, the reduced photoactivation under visible radiation constitutes a major drawback. One of the strategies to overcome this limitation is including plasmonic nanoparticles, such as gold to improve the ability to absorb visible radiation from sunlight. Traditional methods of synthesis include the use of toxic and expensive reagents, here, we propose a green method, using the natural flavonoid quercetin to act as the reducing agent in the deposition of AuNPs on the surface of TiO<sub>2</sub>. The method was optimized, and different loadings of gold were evaluated. The complete characterization of the nanocomposites confirmed an increase in the absorption in the visible wavelength range with increasing concentrations of gold (values ranging between 30 - 70% absorbance). Also, a reduction in the energy band gap from 3.05 to 2.75 eV was calculated. Finally, the photocatalytic efficiency of the synthesized nanocomposites was evaluated for the degradation of the antibiotic ciprofloxacin under UV and simulated sunlight irradiation, verifying a maximum degradation of 86 and 95%, respectively.

## Fabrication and Applications of Nano-structured Graphene with Zigzag Edges

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## Abstract

Graphene is attracting a vast interest both in fundamental research and in industrial applications due to its superior electronic and mechanical properties. However, the research and application of the nano-structured graphene is limited because it is not easy to obtain atomically well-designed edges. Since the edge of graphene shows much different electronic property depending on its structure, either zigzag, armchair, Klein-type or amorphous-like, it is crucial to control the edge structure to fabricate graphene nano-devices reproducibly. Among several kinds of edge structures, the zigzag edge is especially unique because the honeycomb symmetry is broken, and an electronic localized state named zigzag edge state (zES) emerges along the edge. Recently, we have established a technique to fabricate graphene with zigzag edges. The zigzag edge obtained by this technique is found to be not only atomically precise, but also terminated by only one hydrogen atom. Therefore, one can obtain ideal graphene nano-devices with sp<sup>2</sup> bonded carbon atoms to the edge and can expect novel physical characters reflecting the nano-structuring and the zES of graphene. In this presentation, the fabrication, peculiar characteristics, and possible applications of the nano-structured graphene will be discussed. For zigzag graphene nanoribbons (zGNRs) narrower than 20 nm, local density of states which strongly suggest the spin polarization of the zES are observed. On the other hand, for hexagonal networks of the zGNR, named zigzag graphene nano-meshes (zGNMs), unconventional increase of the thermal conductivity by decreasing the nanoribbon width is observed.

## Effective Photoconductivity Modulation for Multifunctional Graphene Photodetectors by Quantum Dots

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## Abstract

Graphene has received wide attention because of its outstanding optical and electrical properties, including high electron mobility, low resistivity, high transmittance, and broad absorption spectrum covering visible to near-infrared light. Hence, graphene is considered to be an auspicious material for advanced photodetectors. Negative photoconductivity (NPC) refers to the effect of a decrease in the conductivity of a photodetector as the device is illuminated. This NPC effect has excellent potential for photoelectric detection, photoelectric switching, and gas detection. Graphene, which is composed of carbon atoms with sp<sup>2</sup> orbitals, is one of the potential materials for constructing NPC devices. In this work, we realize a monolayer graphene photodetector with the NPC effect and the water molecules adsorbed on the graphene are desorbed from the graphene surface under light irradiation. To modulate the NPC effect to the positive photoconductivity (PPC) effect, FAPbI<sub>3</sub> quantum dots acting as a gate bias are introduced on the graphene film. The generated holes can transfer from FAPbI<sub>3</sub> to graphene to increase the conductivity of the graphene channel, resulting in the PPC effect. In conclusion, we offer an effective strategy to modulate the photoconductivity of graphene photodetectors through a simple fabrication process, and the result has great potential to realize sensing systems composed of NPC and PPC effects simultaneously on a chip, which can expand the functions of traditional sensing systems for intelligent Internet of Things applications.

## Re-examination for Nonlinear Behavior of Porous Sandwich Structures Reinforced by Graphene Platelets

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## Abstract

The linear and nonlinear behavior of sandwich structures with porous core reinforced by graphene platelets (GPLs) were re-examined. The graphene platelets reinforced composite (GPLRC) core is assumed to be multilayers with different values of porosity coefficient to achieve a piecewise functionally graded pattern. By introducing an

inhomogeneous model instead of the equivalent isotropic model (EIM), the Young's moduli along with the shear modulus of porous GPLRC core are predicted through a generic Halpin–Tsai model in which the porosity is included. Motion equations are formulated based on the Reddy's third order shear deformation theory. von Kármán nonlinear strain–displacement relationships, shell–foundation interaction and thermal effect are also taken into account. The thermomechanical properties of metal face sheets and the porous GPLRC core are assumed to be temperature dependent. The analytical solution is obtained by applying a two-step perturbation approach. Results reveal that the EIM is invalid for linear free vibration, thermal buckling and postbuckling analyses of sandwich beams with porous GPLRC core and is not suitable for linear free vibration analysis of porous sandwich plates, cylindrical panels, and shells.

## The Berry Benefit - Grape Seed Extract Containing Dentifrice

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### Abstract

A new group of phytochemicals that has been attracting much attention from both the general public and health professionals is a novel drug proanthocyanidin. Grape seed extracts (GSE) are one of the richest sources of proanthocyanidin. GSE increases the expression of anti-inflammatory cytokines and decreased the expression of pro-inflammatory cytokines, thereby reducing the progression of inflammatory diseases such as periodontitis. The aim of the present study was to formulate and evaluate the ability of GSE containing dentifrice to exhibit biologic properties favouring superior oral health status. The test sample consisting of toothpaste containing GSE was formulated and subjected to laboratory investigations. The loaded discs were placed in the Muller-Hinton medium and incubated at 37 °C for 24 h to evaluate its anti-bacterial efficacy against periodontal pathogens. The cytotoxicity study on live cell lines and cell viability was estimated after incubation for 24 h at 37 °C in a 5% CO<sub>2</sub> atmosphere. IL-6 and TNF- $\alpha$  expression by inflammatory cells were tested against RAW cells. The radical scavenging activity was calculated by incubating the test tubes containing the samples in DPPH solution. Comparative analysis of the test sample and control showed significant anti-bacterial (zone of inhibition comparable to positive control), anti-inflammatory (reduced IL-6 and TNF- $\alpha$  expression) and antioxidant efficacy. The current *in-vitro* study provides evidence supporting the efficacy of grape seed extract containing dentifrice in being a potential oral hygiene aid to be used in inflammatory states such as periodontitis.

## Wavelength-dependent Tuning of Thermal and Thermo-plasmonic Response in Aggregates of Porphyrins

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### Abstract

The control of nanoscale thermally activated processes aided by plasmonic resonances has emerged as a cutting-edge research area in the plasmonic field, with diverse applications spanning from medicine to material sciences. In this study, we present an optical and thermal analysis of a porphyrin aggregate using finite element method simulations. The interest in this material is due to the ability to mimic the plasmonic behavior under conditions of strong absorption resonance nearby a spectral region where the real part of the dielectric function is negative. The simulated structure is a 3D right-handed helix, whose geometry reproduces an aggregate of porphyrins, ranging in length from 22,5 to 150 nm. Under illumination by a linearly polarized monochromatic stationary plane wave, the spectral regions of the H- and J-bands are investigated. Due to the different arrangement of transition moments that characterizes the two bands, the optical and thermal behavior observed in steady state are quite different. A

consistent temperature rise is achieved by exciting the H-band, while heating is poor in the J-region. The cause is attributed to the plasmon-like response, which occurs only in the spectral region corresponding to the J-band, where two relaxation mechanisms can be hypothesized to occur: thermal relaxation and plasmon-related optical relaxation. In the spectral region of the H-band, the dielectric function does not allow for plasmonic behavior, resulting in all the energy being dissipated through the thermal channel. The geometry-dependence of the EM field and temperature distributions is also investigated, proving a strong correlation between them.

## Post-acceleration of Electron Bunches from Laser-irradiated Nano Clusters

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### Abstract

The mechanism of acceleration of relativistic attosecond electron bunches after their emission from the interaction of a nanometer-sized droplet with a few-cycle laser is examined by means of three-dimensional particle-in-cell simulations of the light-matter interaction in vacuum. The bunches have attosecond duration and are emitted each half-cycle of the laser following the angular pattern of ponderomotive scattering from an intense laser focus, as it was demonstrated in previous simulation work. Subsequently they are phase-locked with the laser waves and gain energy while traveling in vacuum. Here a spherical geometry is set following not only the initial but also the later times for the evolution of the dynamics of the system. An analytical treatment taking into account a quasi-particle approximation for the bunch and phase calculations for the laser is developed and set for comparison with the three-dimensional picture derived from the PIC simulations. A forward directed particle tracking is set in the code with the purpose of following the bunches' evolution along their path. The analytical equations for the energy gain are in good agreement with the tracking at later times, when the bunches merge in a unique emission pattern with a mean value of the energy. The simulations are shown for the laser intensity of  $5 \times 10^{19} \text{ W/cm}^2$  and the data are collected for intensities up to  $10^{21} \text{ W/cm}^2$ , showing the nonlinear optical mechanism. The emitted bunches hold energy of the order of a few MeVs, and therefore have potential application in the field of energetic X-ray sources.

## Synthesis and Characterization of Photoluminescent Properties, Shape and Size of Gold, Silicon, Copper and Silver Nanoparticles Synthesized via High Energy Ball Milling

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### Abstract

Noble metals gold, silver, silicon, and copper nanoparticles (NPs) were synthesized by Reactive High-Energy Ball Milling of the metal powders in polar solvents. In this work, the mechanical force on the production of nanoparticles ensured the grain size of the NPs would be reduced to sizes of 2 - 20 nm. The crushing of the bulk material increases the surface area of the powder media, facilitating a direct reaction between the metal and ligand. The ball-to-powder ratio in each container for the metal synthesized differed based on the metal synthesized. The ligand L-Cysteine was used in each sample in a 3:1 mol/mol ratio, respectively, so that each nanoparticle synthesized can achieve colloidal stability through electrostatic and/or steric interactions. The NPs generated contained fluctuating sizes and dimensions. This was due to their size, shape, composition, chemical structure, and surface-mediated reaction with L-Cysteine. The synthesized NPs are characterized by X-ray diffraction, scanning electron microscope, Ultraviolet-Visible absorption spectroscopy (UV-Vis), transmission electron microscopy, dynamic light scattering, and room-temperature photoluminescence (PL). The NPs' UV-Vis absorption spectra show the differences between the size

and shape of these materials. Absorptions in the visible regions are due to surface plasmon resonance oscillations in noble metal NPs. The variety of the PL intensity depends on the metal. The results indicate that all samples exhibit different PL emissions in the UV-Vis region (200 - 600 nm). The morphological, physicochemical, and structural characteristics of the synthesized noble metal NPs provide notable functionality, increasing the viability of its utilization for future applications.

## Hydrothermally Synthesized Hierarchical ZnO:Al Nanoscintillator Detector Material for Alpha Monitoring

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### Abstract

We report structural, optical and scintillation properties of well-aligned ZnO based nanoarrays by a facile solution technique. Vertically aligned ultra-dense hierarchical ZnO nanorods showed high quality crystal structure, photoluminescence, and scintillation characteristics. Besides the main precursors such as Zn, ammonium hydroxide and HMTA, the sodium citrate was used as an additive in the solution to control size and shape of the nanoscintillator arrays. Ultraviolet band edge emission (~380 nm) of ZnO based nanoarrays are significantly enhanced and visible emission (~550 nm) originated from surface defects are significantly reduced after annealing samples in a forming gas (10% H<sub>2</sub>N<sub>2</sub>) atmosphere. Hexagonal shaped nanorods are rearranged and are tapered towards the end constituting a nanopencil shape. ZnO nanorods were doped with Al, a group III element, in order to improve the optical and scintillation properties. The as-grown and doped ZnO nanoarray samples were tested in terms of scintillation response using an alpha particle source and a PMT. Pulse height distribution analysis revealed a good scintillation response for as-grown and doped ZnO nanorod arrays. Moreover, the time resolved PL decay time measurements resulted in sub-nanosecond decay time confirming the fast response characteristics of the ZnO nanorod arrays. Nucleation and growth kinetics adopted for this type of material made it possible to grow well-oriented tapered nanoscintillator arrays for alpha particle detection that could be further used for assembly in nuclear detector materials. This work provides a systematic route for size and structure controlled ultrafast, well-oriented ZnO based nanoscintillators by a low-cost and low temperature hydrothermal method.

### Acknowledgements

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## Young Researchers Presentations

### Structural Unit Determination in Silica Nanoparticles Using Infrared Micro-reflectance Spectroscopy

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#### Abstract

Characterization of the structural units of glasses is an essential part of amorphous materials research, with implications for all kinds of properties, from chemical reactivity to crystallization. The relative proportions of units in silicate glasses can be quantified by magic-angle spinning <sup>29</sup>Si nuclear magnetic resonance (MAS-NMR) spectroscopy. Simpler alternatives include Raman spectroscopy, which is affected by luminescence, and infrared spectroscopy, which requires the use of deconvolution techniques to resolve structural information. Furthermore, if the materials under study are nano-sized, extracting quantitative information about their structure from infrared spectroscopy is even more complicated, as the effect of porosity needs to be taken into account through so-called effective medium theories. In this work, silica nanoparticles have been investigated using infrared micro-reflectance spectroscopy and nuclear magnetic resonance spectroscopy. Colloidal silica was chosen because of its chemical and structural simplicity, with only H atoms acting as modifiers of the glass network. The use of micro-reflectance, instead of transmittance or attenuated total reflectance, allows for greater accuracy and reproducibility between samples. The results are analyzed through the Landau-Lifshitz-Looyenga effective medium approximation and a robust deconvolution procedure for the absorption bands, in which each component is attributed to a microscopic origin. Excellent agreement is found between infrared and NMR spectroscopies, lending credence to this technique as a simple and accurate, albeit less precise, alternative for structural unit quantification. Because of the generality of this technique, it could be easily extended to other silicate nanomaterials.

### Atomic Movement Mechanisms of Plasticity-induced Phase Transitions in Gradient Nanostructured High-entropy Alloys

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#### Abstract

Dual- or multi-phase materials have shown promise in achieving co-deformation cooperative effects, resulting in significant improvements in the strength-ductility synergy and other mechanical properties. Notably, the combination of strength and ductility in medium/high-entropy alloys (M/HEAs) can also be significantly enhanced through plasticity-induced solid-to-solid phase transitions. However, the atomic movement mechanisms underlying these phase transitions remain poorly understood. In this study, we investigate two distinct phase transitions: bcc → hcp and fcc → hcp → bcc, observed in bcc-based TiZrHfTa<sub>0.5</sub> and fcc-based Fe<sub>45</sub>Mn<sub>35</sub>Cr<sub>10</sub>Co<sub>10</sub> HEAs, respectively, receiving severe plastic deformation. Through atomic observations, we elucidate the atomic movement mechanisms governing these phase transitions. In the bcc → hcp phase transition of TiZrHfTa<sub>0.5</sub> HEA, we identify two primary atomic movement mechanisms: cooperative atom shuffling and gliding of partial dislocation dipoles. This phase transition contributes to the excellent tribological performance of the alloy. Additionally, we engineer a phase transformation following the fcc → hcp → bcc sequence in the gradient nanostructured surface layer of Fe<sub>45</sub>Mn<sub>35</sub>Cr<sub>10</sub>Co<sub>10</sub> HEA using a surface severe plastic deformation technique. The atomic movements involved in the fcc → hcp → bcc transition occur in two steps. The first step, fcc → hcp, is accomplished by Shockley



partial dislocations on alternating (111) fcc planes, while the second step, hcp  $\rightarrow$  bcc, involves the combination of Shockley partial dislocation dipoles on both sides of the (0001) hcp phase and atomic shuffling along the  $[11\bar{2}]_{\text{fcc}} // [1\bar{1}0]_{\text{bcc}}$  directions.

### Acknowledgements

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## Nanostructures and Strengthening Mechanisms in Additive Manufactured Coherent Nanoprecipitation Containing High Entropy Alloys

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### Abstract

Nanoprecipitation hardening has been proven effective in enhancing the mechanical properties of single-phase high-entropy alloys (HEAs). The performance of coherent nanoprecipitation-reinforced HEAs relies on their hierarchical microstructures, especially the distribution and morphology of nano-precipitates. Although prior studies have highlighted the advantages of combined additive manufacturing (AM) and thermal mechanical processing for producing high-performance HEAs, the resulting enhancements in mechanical properties were limited primarily to grain refinement. This study employs a one-step cold-rolling process to modify the microstructural characteristics of the coherent nanoprecipitates and further strengthen the as-AMed HEA. AM is effective in fabricating grain-refined alloys with elemental nanoscale heterogeneity. Thus, the as-AMed HEA can serve as a suitable primary material state for further thermal-mechanical processing and facilitate the radical change in nanoprecipitation behavior. Modified high-density coherent precipitates divide the FCC matrix into extremely fine nanoscale channels, leading to a significant dynamic Hall-Petch effect during subsequent deformation. Additionally, multiple nanoscale strengthening mechanisms were activated upon deformation, including stacking fault networks and heterogeneity-induced plasticity. Benefiting from the high compositional complexity, the nano-precipitates in this HEA had high deformability and rendered the alloy super-high tensile performance. By carefully controlling the ratio and size distribution of the continuous and discontinuous nanoprecipitates, the resulting alloy achieves a superior yield strength of approximately 1.5 GPa. A comprehensive investigation was conducted to elucidate the effect of the modified nanostructures in the alloy and the contributions of alternative strengthening mechanisms.

## Time-scale Investigation with Modified Phase Field Crystal Method

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### Abstract

We present a two-timescale modified phase-field crystal model to examine crystal plasticity. Building on earlier versions, we build strain and strain-rate couplings to the density dynamics. The non-linear additions provide tunable parameters for controlling dislocation climb versus glide, as well as phonon softening mechanisms. A short-wavelength dampening is also introduced to account for phonon scattering and thermoelastic dissipation processes. Finally, we discuss a novel semi-implicit numeric scheme for efficient simulation of this model, which also serves as a generalization of the commonly used Fourier pseudo-spectral method. The technique gives rise to unconditionally stable dynamics with simple numeric implementation requirements. We shall also describe our recent work on phase field crystal models to quantitatively investigate growth structures in conditions amenable to additive manufacturing.

## Study on the Adsorption Properties of Hydrochloric Acid Doped Microporous Conjugated Polyaniline for Hg<sup>2+</sup>

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### Abstract

Mercury (Hg<sup>2+</sup>) is a typical heavy metal pollutant that poses serious risks to human health. Currently, adsorption, as a physical method, favored for its simplicity and low cost. Among various adsorbents available, polyaniline has garnered extensive research interest owing to its reversible doping and de-doping characteristics, low price, and safety. However, the one-dimensional structure of polyaniline limits its specific surface area, leaving ample room for improvement in its adsorption performance. Conjugated microporous polymers, a type of three-dimensional network material, have attracted considerable attention due to their combined extended  $\pi$ -conjugation with a permanently microporous skeleton. We firstly propose a strategy to tune the adsorption selectivity of CMPA towards Hg<sup>2+</sup> by using a simple doping treatment with inorganic acids. These doped materials were used to adsorb Hg<sup>2+</sup>, and the results indicated that HCl-doped CMPA exhibited significantly higher adsorption performance compared to the undoped material and other acid-doped adsorbents, warranting further investigation. The Langmuir adsorption capacity of HCl-CMPA was determined to be 832.8 mg/g, surpassing most previously reported materials. This outstanding value is even 175% higher than its parent matrix without HCl modification, showing that HCl-doped microporous conjugated polyaniline have promising adsorption capacity towards Hg<sup>2+</sup>.

## Targeted Chemical Modification for Controlled Supramolecular Assembly

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### Abstract

Targeted chemical modification for controlled supramolecular assembly understanding and controlling the properties of functional materials is a challenging task [1, 2]. One way of achieving this goal is by targeted alteration and modulation of the intramolecular interactions between the compounds, which can be realized by adding or converting functional groups. We use different classes of molecules to demonstrate this principal e.g., perylene diimides, owing to their strong  $\pi$ - $\pi$  interactions and interesting optoelectronic properties [3, 4]. Addition of functional groups capable of hydrogen bonding (e.g., amide and urea moieties) is also utilized to promote further supramolecular interactions [5]. Those modulated interactions between the molecules can then be used to tailor the properties to fit the desired application. With these principles established, we show further examples of chemical modifications of functional polymer systems; the resulting compounds are then thoroughly assessed to obtain deeper insight into the structure-properties-function relationship for novel applications. Specifically, we are now in the process of establishing design rules for the targeted preparation of functional materials tailored for application as bio-adhesives.

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## Generation and Enhancement of Currents and Magnetic Fields in a Two-dimensional Quantum Ring Using Short Electromagnetic Pulses

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### Abstract

We present the study of the SiGe quantum ring modeled by an anharmonic axially symmetric potential with a centrifugal core in the effective mass approximation. We show how the femtosecond laser pulses (FLPs) can be used efficiently for controlling the induced current and magnetic field. We have compared the strength of induced currents and magnetic fields with and without a pulsed laser which shows a substantial change. The spin-orbit interaction (SOI) and Zeeman energy show a massive impact on the generation and enhancement of these induced current and magnetic fields. These induced currents and magnetic fields have many applications in interdisciplinary areas. We have shown that the SOI presence with the FLP fields while competing with the confinement strength lowers the strength of the induced current and field.

## High-resolution Study of Changes in Morphology and Chemistry of Microphase Separated PS-*b*-PMMA Thin Films After Selective Removal of PMMA

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### Abstract

Block copolymer lithography (BCP) is one of the emerging techniques to produce nanostructured lithography masks with feature sizes in the single-digit nanometer regime. These masks are obtained by a microphase separation of the BCP consisting of two blocks of immiscible polymer species, A and B, which are covalently bond in a BCP chain. The microphase separation results in, e.g., periodically arranged cylinders or lamellae of A in a matrix of B. Among the BCPs, polystyrene-*b*-polymethylmethacrylate (PS-*b*-PMMA) is the most used. Recent studies reveal an intermixing between PS and PMMA across the microdomain interface after microphase separation. However, the abruptness of the BCP microdomains is crucial, when BCPs are considered for high-resolution lithography. Further processing steps to obtain a BCP mask typically include the selective removal of PMMA. Therefore, detailed investigations of the PS mask wall morphology after selective removal are mandatory.

To give insights into changes in morphology and surface chemistry, we compare the mask features after PMMA removal by either dry or wet etching using analytical scanning transmission electron microscopy as well as X-ray photoelectron spectroscopy and polarization modulated infrared reflection absorption spectroscopy. In addition, PS-*co*-PMMA random copolymer brushes which are frequently used as substrate functionalization layers aiding controlled BCP self-assembly are investigated to understand the impact of the dry and wet etching processes. These insights will allow to understand each processing steps and enhance the precision of features created by block copolymer lithography.

## Solid Phase Synthesis of Molecularly Imprinted Polymers Using Different Rigid Substrates

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### Abstract

Molecularly Imprinted Polymers (MIPs) are synthetic receptors produced from polymers in the presence of a template molecule. NanoMIPs are fabricated by copolymerizing functional monomers, cross-linkers, and a template molecule. Structurally and electrostatically complementary vacancies are generated upon removing the template. NanoMIPs use a “lock and key” method to selectively bind their molecule, like natural antibody-antigen systems. They facilitate biological receptors specificity and selectivity in an inexpensive and durable way. MIP synthesis involves immobilizing a template molecule on a solid substrate – glass beads, polymerizing with functional monomers and cross linkers, which subsequently includes extraction of template molecule to leave imprinted cavities for target-specific rebinding. Tryptophan, an amino acid based nanoMIPs was synthesized using 3 different solid substrates, the traditional glass beads of diameter 75 - 90  $\mu\text{m}$  whereas the other two substrates being glass slides (GS) and glass covers (GC). The average size of tryptophan nanoMIPs synthesized on glass beads are 250 nm, whereas on GS and GC it varies in the range of 60 - 100 nm. To the best of our knowledge, this is the first study using GS and GC solid substrates for synthesizing nanoMIPs leveraging with the lowest possible size achieved in comparison to the traditional method. It is known that smaller sized nanoMIPs have larger surface area and faster binding kinetics resulting in higher sensitivity for target molecule detection and also exhibit reduced non-specific binding. Our future work is targeted towards mobilising these MIPs onto gold nanoparticle-based SERS substrate for further analysis of binding affinity.

## Luminescent and Electrical Properties of Silver Nanoparticles Embedded in Thiourea-grafted Pectin

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### Abstract

Thin films of pectin grafted with thiourea and epichlorohydrin were prepared and silver nanoparticles were loaded onto them. Their electrical properties were evaluated by electrical impedance for determination of their ionic conductivities, while the electron conductivities, and band gap energy, were estimated by Tauc plot using the diffuse reflectance measurements. From results obtained can be inferred that the ionic conductivity of pectin is decreased due to the grafting polymerization process, but the incorporation of silver nanoparticles is advantageous for the ionic conductivity of the nanocomposite. Meanwhile, electrical conductivity, both the grafting polymerization process and the silver nanoparticles embedding increase the band gap energy. In addition, an emission study led to the observation of a notable increase of the luminescent properties of prepared films.

## Symposium II: Future Biomaterials-Biomedical, Medicine and Other Applications

### Featured Presentations

#### Magnetoplasmonic Nanocapsules as Wirelessly Controlled Nanotherapies

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#### Abstract

Advanced nano-biomedical applications have been traditionally based on chemically synthesized inorganic nanoparticles. Here we present a novel type of structure especially suited for diverse biomedical uses: magnetoplasmonic nanodomains. The nanodomains are composed of magnetoplasmonic semishell deposited onto 100 - 200 nm diameter polymer beads. The very high plasmonic absorption of the nanodomains in the near infrared is used for very efficient local optical heating for cancer treatment. The nanodomains magnetic character allows to remotely manipulate them to easily regulate the level of photo-hyperthermia. Moreover, their asymmetric shape exhibits strong optic and magnetic anisotropies. Thus, rotation of the nanodomains using alternating magnetic fields can be tracked optically using their different absorption depending on the orientation. Since the rotation of the nanoparticles depends strongly on the viscosity of the medium, which in turn depends on the temperature, the optical tracking of the rotation can be used to accurately determine the local temperature change around nanodomains, allowing *in-situ* tracking the photo-hyperthermia treatments. The same nanodomain concept can be extended to drug delivery, where the semishell allows for remote control of the nanocapsule, or MRI tracking of the beads. This concept of magnetoplasmonic nanocapsules loaded with paclitaxel drug has enabled complete eradication of the tumors *in vivo* in mice by combining magnetic concentration and photothermal actuation, using a drug concentration between 200 and 500-fold lower than the therapeutic window of the free drug. We have extended this nanocapsules concept to combine simultaneous photodynamic and photothermal therapies, or enhanced antibiotic effects.

#### Magnetic Nanomotors to Navigate in Complex Environments

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#### Abstract

Nano/micromotors (or swimmers) are a class of active matter that can convert an input energy into kinetic energy to outperform Brownian motion. Among the possible options, magnetic fields are a reliable source to propel motors since they can be easily tuned and present no risks to living organisms if applied in a biological context. One of the major challenges regarding motors and biomedicine is to use the motors' power to reach cytosolic placement, i.e., to avoid remaining trapped in lysosomes. Theoretical approaches have been conducted to identify the interaction between particles and cell membrane models. However, the experimental validation of these models is still limited. Here, we use magnetic micromotors to assess their interaction when navigating in an environment that contains giant unilamellar vesicles as simple mimics of cell membranes. With the aim to understand the requirements for motors to cross the membranes, different parameters were considered, such as motor size and coating, lipid membrane composition, density of the medium and the magnetic field strength. Taken together, we could identify fundamental design criteria for motors that exhibit sufficient power to cross an important biological barrier i.e., lipid bilayers.



## Multifactorial Drug Delivery System Comprising Gold Nanoparticles Assembled with $\alpha$ -Synuclein

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### Abstract

$\alpha$ -Synuclein ( $\alpha$ S) is an amyloidogenic protein responsible for the Lewy body formation found in Parkinson's disease. Based on its unique unit-assembly mechanism in which  $\alpha$ S oligomers are assembled into amyloid fibrils by acting as accreting units upon their structural alteration in the presence of external stimuli such as shear force, heat, and solvents, gold nanoparticles (AuNPs) have been fabricated into hierarchical structures such as 1D nano-chains, free-standing 2D films, and 3D microcapsules. In particular, the  $\alpha$ S-AuNP microcapsules could be employed to tackle tumor heterogeneity by integrating various cytotoxic agents. Upon proteolysis as a pathological indicator, both hydrophobic drugs and inverted micelles carrying hydrophilic drugs inside are released from the microcapsules framed with porous inner skeleton made of a biocompatible polymer of poly(lactic-co-glycolic acid) which has been introduced to prevent the collapse of microcapsules and thus save the micelles from their coalescence. The heterogeneous cancer cells are then eliminated all together by both chemical and physical means, which includes various drugs specifically delivered into the cells, membrane destabilization caused by the inverted micelles, and photothermal effect of the AuNP microcapsule remnants engulfed by the cells. Therefore, the multifactorial cargo delivery system capable of handling the tumor heterogeneity has been considered as a promising future biomaterial as Nano-Bio-Fusion Product.

## Polymeric-based Nanomedicines Targeting Brain Lipid Metabolism: A Next Generation Therapy for Neuron-related Diseases

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### Abstract

The alarming global increase of neuron-related diseases such as neurodegeneration, obesity and related complications suggest an urgent need for new therapeutic strategies. Pharmacotherapy alone or in combination with either lifestyle modification or surgery, is consistent in maintaining a healthy body weight, and preventing progression to obesity-related diseases. However, anti-obesity drugs are limited by non-specificity and unsustainable weight loss effects. Therefore, further research is needed to develop new preventive and treatment approaches to regulate energy homeostasis. Targeting brain lipid metabolism is a promising strategy to regulate energy balance and fight metabolic diseases tightly controlled by brain cells. The development of stable platforms for selective delivery of drugs, particularly to the hypothalamus, is a challenge but a possible solution for these diseases. Attenuating fatty acid oxidation in the hypothalamus via carnitine palmitoyltransferase 1A (CPT1A) inhibition leads to satiety, but this target is difficult to reach *in vivo* with the current drugs. We propose using an advanced crosslinked polymeric micelle-type nanomedicine that can stably load the CPT1A inhibitor C75-CoA for *in vivo* control of energy balance. Central administration of the nanomedicine induced a rapid attenuation of food intake and body weight in mice via regulation of appetite-related neuropeptides and neuronal activation of specific hypothalamic regions driving changes in the liver and adipose tissue. This nanomedicine targeting brain lipid metabolism was successful in the modulation of food intake and peripheral metabolism in mice. This investigation might contribute to the development and validation of a new generation of nanomedicine-based approaches targeting brain cells.

## Using Core Shell Extrusion to Achieve Functional Tissue Engineering Blood Vessels

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### Abstract

Blood vessels are key elements to provide tissues and organs with nutrients and oxygen. Short after tissue damage, the formation of blood vessels are critical for successful tissue regeneration. Up to now, several methods have been used to reproduce blood vessel-like structures, although they are generally complex with elevated costs. The aim of this work is to develop a multilayered hollow hydrogel-based fiber to mimic the architecture of a blood vessel. To this end, we used the extrusion technique using a core-shell nozzle, utilizing alginate and collagen as a main hydrogel composition. Human umbilical vein endothelial cells (HUVEC) and human smooth muscle cells (hSMCs) were encapsulated in the core and in the shell, respectively. This extrusion method allowed the production of a tissue engineered blood vessel-like (TEBV) structure in the range of arteries with low cost and presenting high homogeneity between TEBV constructs. Furthermore, TEBVs constructs were able to encapsulate HUVEC and HASMC, allowing their survival (over 90%) and proliferation within it. Additionally, HASMC showed a perpendicular alignment, resembling the alignment of smooth muscle cells in native arterial blood vessels. On the other side, HUVEC cells presented parallel alignment only in the initial cell culture period. Further experiments require perfusion of these TEBV-like structures in order to induce the proper cell alignment and maturation and functionality of the construct.

## Carbon Nanostructure Derivatives as Fillers in Scaffolds for Tissue Engineering and Regenerative Medicine

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### Abstract

Carbon nanostructures (CNSs), including carbon nanotubes (CNTs) and graphene-based materials, can be employed as fillers in a biocompatible polymer phase, combining the properties of the two constituents to act as functional materials for applications including medical devices, tissue engineering and biosensing.

Functionalizing CNSs with suitable organic groups is an effective strategy to increase the affinity between the two phases, maximizing the desired effects while minimizing the loading and preventing cytotoxicity of the filler.

We synthesized CNT derivatives that can be efficiently dispersed in poly(l-lactic acid) and the resulting composites have been processed in the form of films and electrospun nanofibers, to obtain scaffolds that are able to promote neuronal growth and differentiation starting from either SH-SY5Y human neuroblastoma cells or human circulating multipotent stem cells from peripheral blood, in the latter case even in the absence of exogenous neurotrophins.

Extending the approach to other CNSs, such as reduced graphene oxide (RGO) and carbon nanohorns (CNHs), showed how different dimensionalities give rise to different properties within the composite. Such observation opens the possibility to design scaffolds for the regenerative medicine of different tissue types. Indeed, we observed that, while nanocomposites based on highly conductive CNTs boost neuronal differentiation, less conductive CNH and RGO fillers enhance the expression of myogenic markers.

An innovative surgical implant designed for nerve regeneration has been prepared by dispersing water soluble CNT derivatives in an oxidized polyvinyl alcohol hydrogel matrix. *In vivo* tests show promising results in terms of biocompatibility and effectiveness in restoring.

## 3D Printable Nanocomposite for Bioinspired and Functionalized Microneedles

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### Abstract

This work presents a functionalized polymeric nanocomposite developed to produce printable microneedles in two hierarchical size scales for drug delivery: the first one, bioinspired in the microstructures of urticating hairs of sting nettle (*Urtica dioica* L.), characterized by their curved shape, and a second one, to cover the first, constituted of multi-walled carbon nanotubes (MWCNT) oriented as nanoneedles for virus inactivation. The bioinspired microneedles (BMN) are printed using high-resolution MSLA printers, stereolithography with 8K LCD as a digital mask, with 405 nm radiation for photopolymerization. The produced BMNs present bactericidal properties due to the self-growth of Ag<sup>0</sup> nanoparticles growth *in situ* by photoreduction during this 3D printing process. Also, the BMNs present an increased mechanical strength and thermal stability due to this photo-reduced nanometric phase growth during the printing process. The synthesized resin with and without silver dissolved completely in simulated body fluid, making it suitable for drug delivery by BMN dissolution. SEM confirmed crystal-like microstructures, EDX mapping showed silver on the surface, and AFM analysis revealed differences in roughness in the presence of silver. FTIR-ATR and UV-Vis spectroscopy were used to study the chemical composition and metallic silver in the nanocomposite. MWCNT alignment through electric fields has possibilities for further investigation. The developed resin is suitable for printing medical devices with bactericidal effects, which is important for transdermal drug delivery and self-decontamination capabilities.

## [1]Benzothieno[3,2-b][1]-benzothiophene (BTBT)-peptide Hybrid Hydrogels for Bioelectronics

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### Abstract

The conjugation of small molecule organic semiconductors (OSCs) with self-assembling peptides is a powerful tool for the fabrication of supramolecular soft materials for organic electronics and bioelectronics. Herein we present a hybrid system in which [1]benzothieno[3,2-b][1]-benzothiophene (BTBT), a popular OSC with a striking high charge carrier mobility, has been conjugated to a self-assembling amphipathic peptide. We show the formation of pH-triggered self-supporting hydrogels. Using a pool of spectroscopic techniques, we demonstrate that supramolecular long range 1D structures are enabled by the synergistic action of both  $\beta$ -sheet peptide formation and strong  $\pi$ - $\pi$  stacking between BTBT chromophores. Moreover, the material showed a conductivity up to  $1.6 (\pm 0.1) \times 10^{-5} \text{ S cm}^{-1}$  when deposited on gold interdigitated electrodes.

## Suitability of Microwave Radiation for the Synthesis of Bioactive Glasses

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### Abstract

It is well known that the use of microwaves results in rapid and uniform heating (no selective heating of the surface), energy saving process (low power consumption in order to reach low to moderate working temperatures), higher yield and shorter preparation time, lower processing cost, small narrow particle size distribution and high purity. Based on that, the main objective of this work was to synthesise bioactive glasses by a hydrothermal chemical route assisted by microwaves.

The bioactive glass 58S (58% SiO<sub>2</sub>, 33% CaO and 9% P<sub>2</sub>O<sub>5</sub> in wt.%) has been chosen as the working composition. Aqueous-based solutions were prepared employing different alkoxides and salts. Then, the sols were heated using a microwave digestion system (MW Ethos One, Milestone) testing different temperatures and pressures. Finally, the resulting material was crushed to a powder and stabilised by a thermal treatment using a lab-made microwave sintering furnace. Moreover, the same glass was synthesised by the sol-gel method, stabilized using a conventional furnace and taken as reference. All glasses were immersed in simulated body fluid up to 14 days following a standard protocol. Before and after immersion, the glasses were characterised by means of scanning electron microscopy, X-ray diffraction, energy dispersive X-ray spectroscopy, and Fourier-transform infrared spectroscopy.

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## Two-photon Fluorescent (nano)probes for a Versatile Intracellular Detection and Quantification of Nitric Oxide

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## Abstract

Nitric oxide (NO) is involved in numerous biological processes, playing an important role in the regulation of diverse physiological and pathophysiological mechanisms of the cardiovascular, nervous, and immune systems; and alterations in the intracellular NO concentrations have been linked to a large number of diseased states. Considering the significant role that NO plays in important biological functions, the development and improvement of methods to detect and quantify intracellular NO are essential to further our understanding of the biological roles of NO.

This contribution will present near infrared excitable (nano)probes for the intracellular detection and quantification of NO that take advantage of the high photostability, high biological tissue penetration and minimal photodamage associated with this long-wavelength excitation. The (nano)probes are broadly applicable and are able to detect and potentially quantify NO levels in an extensive range of cellular environments including endogenous NO in RAW264.7γ NO<sup>-</sup> macrophages and THP-1 human leukemic cells, and endogenous and exogenous NO in endothelial cells. The (nano)probes accumulated in the acidic organelles of the tested cell lines showing negligible toxicity. Importantly, the nanomaterials showed potential to quantify intracellular NO concentrations in MDA-MB-231 breast cancer cells. Based on their excellent sensitivity and stability, and outstanding versatility, the developed (nano) probes can be applied for the spatiotemporal monitoring of *in vitro* and *in vivo* NO levels.

## A Facile Approach for Producing Polypyrrole Microcapsules and Their Application in Bio-electrochemical Sensing

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## Abstract

We present a facile and rapid approach for producing polypyrrole microcapsules that offers several advantages over alternative methods. The proposed method is compatible with both vortex mixers and microfluidic chips, enabling the efficient generation of microcapsules of very different sizes. Additionally, the chip geometry can be modified to some extent, enabling size control over the resulting sub-micron particles. The capsules generated exhibit excellent stability in solution and can be used in high-performance electrochemical devices. Our method also avoids the need for surfactants or organic solvents, enabling new possibilities in biosensors, electronics, and molecular delivery.

To illustrate the application of the microcapsules generated, we incorporated them onto screen printed electrodes, resulting in a remarkable increase in their electroactive surface area and capacitance. By further modifying the electrodes with glucose dehydrogenase, we developed glucose biosensors. The introduction of polypyrrole microcapsules significantly expanded the dynamic range of the glucose sensor, achieving a three-fold wider linear range compared to sensors without the capsules. The glucose sensor operates at a constant applied potential of 0.20 V vs Ag/AgCl (3 M KCl) in an air-equilibrated electrolyte. The sensor exhibits a linear response from 1.0 to 9.0 mM glucose, with a sensitivity of  $3.23 \mu\text{A}\cdot\text{cm}^{-2}\cdot\text{mM}^{-1}$  ( $R^2 = 0.993$ ). The limit of detection achieved is 0.09 mM, and the sensor preparation is highly reproducible (RSD = 3.6%).

## Safety Assessment of 2D Materials at the Skin Level

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### Abstract

Safety issues of 2D materials (2DM) for human health are mainly associated with an occupational exposure during their production process along their life cycle. In this context, cutaneous contact is certainly one of the most important exposure routes to these materials. In addition, technological applications implying a direct skin contact are already available for some of them: beyond graphene-related materials, several other 2DM are currently exploited in this sector, such as transition metal dichalcogenides (such as  $\text{MoS}_2$  and  $\text{WS}_2$ ), hexagonal boron nitride, MXenes and black phosphorus.

In this view, we have characterized the hazard posed by some of these 2DM using advanced *in vitro* skin tools, such as a 3D model of human epidermis. The analysis did not allow only to gain knowledge on the main adverse outcomes possibly exerted at the skin level (i.e., irritation and corrosion) by these materials, but also allowed to shed light on their mode-of-action at the epidermal level.

## Preclinical Development and Evaluation of Formulated Fish Peptides to Support Management of Hypertension

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### Abstract

The angiotensin-converting enzyme inhibitory peptides, Ile-Pro-Pro (IPP) and Leu-Lys-Pro (LKP), both isolated from fish, have shown antihypertensive activity. However, the oral bioavailability of both peptides is low due to poor uptake in the gut. IPP and LKP were formulated into nanoparticles using chitosan via ionotropic gelation and then coated with zein. Following addition of zein, a high encapsulation efficiency of 80% was obtained for the nanoparticle. In simulated gastric fluid, 20% cumulative release of the peptides was achieved after 2 h, whereas in simulated intestinal fluid, ~90% cumulative release was observed after 6 h. Higher colloidal stability (39 - 41 mV)



was observed for the coated nanoparticles compared to uncoated ones (30 - 35 mV). *In vitro* cytotoxicity studies showed no reduction in cellular viability of human intestinal epithelial Caco-2 and HepG2 liver cells upon exposure to nanoparticle components. In spontaneously hypertensive rat studies, oral delivery of the nanoparticles exhibited an enhanced antihypertensive effect (for 8 h) of both IPP and LKP with a longer therapeutic effect compared to free peptides. The data was similar to the standard commercial therapeutic, captopril. This suggests that the nanoparticle provided increased intestinal absorption and sustained release to achieve prolonged hypotensive effects of both peptides *in vivo*. Oral administration of IPP/LKP nanoparticles might be a potential strategy for hypertension treatment in the future.

## Biomimetic Multifunctional Materials

Lluís Oliver-Cervelló<sup>1,2</sup> and Carlos Mas-Moruno<sup>1,2\*</sup>

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### Abstract

Mimicking bone extracellular matrix is paramount to develop novel biomaterials for bone tissue engineering. In this regard, the combination of integrin-binding ligands together with osteogenic peptides represents a powerful approach to recapitulate the healing microenvironment of bone. In the present talk, we will discuss the synergistic effects achieved by chemically controlling the combination of the cell adhesive peptide RGD with a peptide derived from bone morphogenetic protein-2, the DWIVA sequence. Preliminary studies showed the capacity of the peptides to engage in integrin-growth factor signaling [1], and their potential to promote human mesenchymal stem cells adhesion and osteogenic differentiation, as well as formation of new bone *in vivo* on titanium implants [2]. Subsequently we will explore the translation of this strategy to protease-degradable polyethylene glycol-based hydrogels, thus expanding the scope of these peptides to more complex 3D systems.

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### Acknowledgements

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## Nanoactuators for Therapy and Diagnosis

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### Abstract

In the last decades, inorganic nanoparticles have been steadily gaining more attention from scientists from a wide variety of fields such as material science, engineering, physics, or chemistry. The very different properties compared to that of the respective bulk, and thus intriguing characteristics of materials in the nanometre scale, have driven

nanoscience to be the centre of many basic and applied research topics. Moreover, a wide variety of recently developed methodologies for their surface functionalization provide these materials with very specific properties such as drug delivery and circulating cancer biomarkers detection. In this talk we describe the synthesis and functionalization of magnetic and gold nanoparticles as therapeutic and diagnosis tools against cancer.

Gold nanoprisms (NPRs) have been functionalized with PEG, glucose, cell penetrating peptides, antibodies and/or fluorescent dyes, aiming to enhance NPRs stability, cellular uptake, and imaging capabilities, respectively. Cellular uptake and impact were assayed by a multiparametric investigation on the impact of surface modified NPRs on mice and human primary and transform cell lines. Under NIR illumination, these nanoprobe can cause apoptosis. Moreover, these nanoparticles have also been used for optoacoustic imaging, as well as for tumoral marker detection using a novel type of thermal ELISA and LFIA nano-biosensor using a thermosensitive support.

## Promoting Effect of a Calcium-responsive Self-assembly $\beta$ -sheet Peptide on Collagen Intrafibrillar Mineralization

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### Abstract

Recently, a *de novo* synthetic calcium-responsive self-assembly  $\beta$ -sheet peptide ID8 (Ile-Asp-Ile-Asp-Ile-Asp-Ile-Asp) has been developed to serve as the template inducing hydroxyapatite nucleation. The aim of this study was to evaluate the effect of ID8 on intrafibrillar mineralization of collagen making full use of its self-assembly ability. The mineralization experiments were carried out *in vitro* on both bare type I collagen and fully demineralized dentin samples. The calcium-responsive self-assembly of ID8 was revealed by circular dichroism spectrum, 8-anilino-1-naphthalenesulfonic acid ammonium salt hydrate assay, attenuated total reflection-Fourier transform infrared spectrum (ATR-FTIR) and transmission electron microscope (TEM). Polyacrylic acid (450 kDa) with a concentration of 100 mg/L was selected as the nucleation inhibitor based on the determination of turbidimetry and TEM with selected area electron diffraction (TEM-SAED). The results showed that collagen intrafibrillar mineralization was significantly promoted with the pretreatment of self-assembly ID8 detected by TEM-SAED, SEM, X-ray diffraction, and ATR-FTIR. The pretreatment of collagen utilizing self-assembly ID8 not only enhanced intermolecular hydrogen bonding, but contributed to calcium retention inside collagen and significantly increased the hydrophilicity of collagen. These results indicated that peptides with self-assembly properties like ID8 are expected to be potential tools for biomimetic mineralization of collagen.

## New Approaches to Inhibit miRNAs in an Atherosclerosis Pre-clinical Model

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<sup>2</sup>CIBER Diabetes and Associated Metabolic Diseases (CIBERDEM), Spain

### Abstract

It is known that several microRNAs (miRNAs) have an important regulatory role during the different stages of the atheroma plaque formation. In preclinical studies, the regulation of its expression has been shown beneficial outputs in the treatment of atherosclerosis. Thus, the therapeutic targeting of miRNAs represents an attractive approach for the treatment of atherosclerosis in preclinical and clinical studies. Different approaches have been undertaken to decipher the potential of miRNA therapeutics. To repress pathological miRNAs or over-express protective miRNAs, miRNA inhibitors or miRNA mimics, respectively, have been employed. Despite significant achievements in the field, cellular uptake, the potential need for multiple doses to achieve the desired effect, biodistribution, the ability to target a specific tissue or cell, the unpredictable and unwanted side effects and toxicity still remain the major limitations for miRNA-targeting therapies. All of these challenges have emphasized the need to develop more

efficient delivery systems for miRNA therapeutics in the context of atherosclerosis. Thanks to the development of nanotechnology in the molecular biology field, novel delivery miRNA-base therapies have emerged. The use of an innovative therapeutic approach for targeting miRNAs *in vivo* using a pH low-insertion peptide it might be of interest. Moreover, the incorporation of miRNA into sHDL with therapeutic purposes is promising. Thus, a miR-sHDL could be an innovative technique and a powerful vehicle tool for searching overexpression or inhibition of key miRNAs in atherosclerotic plaques.

## Crystalline Titania Formation on Ti-based Dental Implants and its Role in Biocompatibility

Benedetta Albini<sup>1\*</sup>, Pietro Galinetto<sup>1</sup>, Maddalena Patrini<sup>1</sup>, Giampiero Pietrocola<sup>2</sup> and Saturnino Marco Lupi<sup>3</sup>

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### Abstract

Titanium is the most used material in the dental implant market since it displays mechanical and physical characteristics that lead to high survival and successful osseointegration rates. However, titanium is a bioinert material, thus the increased biocompatibility is imparted by an amorphous nanometer layer of TiO<sub>2</sub> [1], that naturally and easily formed on the external surface. The highly defective titanium oxide layer can be ordered after high temperature heating or anodizing treatments, leading to the formation of a crystalline phase (anatase or rutile). In this regard, a crucial issue is to deeply understand the development of TiO<sub>2</sub> phases as a function of manufacturing processes and to what extent its crystallinity relates to its biocompatibility. Raman spectroscopy (RS), based on the inelastic scattered of light upon application of a monochromatic incident source, is a well-established technique to monitor TiO<sub>2</sub> formation. Moreover, RS allows to characterize TiO<sub>2</sub> in term of crystal, crystalline quality and eventually nanoscale morphology. The aim of this research is to carefully characterize by means of RS investigation, the surfaces of different implants realized with the most diffused Ti-based materials: commercially pure titanium implants and Ti-6Al-4V alloy [2, 3]. The RS results have allowed to evaluate the effectiveness of the different investigated surface treatments by extracting a semi-quantitative parameter that relates to the titania crystallinity. The RS evidence has been corroborated, explained, and complemented by scanning electron microscope with energy dispersive X-ray probe, X-ray fluorescence measurements. All these data are discussed considering antibacterial activity tests.

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## Young Researchers Presentations

### Bilayer Hydrogels for Improved Oocyte Maturation

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<sup>2</sup>Regional Institute for Applied Scientific Research (IRICA), UCLM, Spain

#### Abstract

In the field of assisted reproductive technologies, oocyte *in vitro* maturation (IVM) is emerging as a promising solution to overcome the limitations associated with traditional ovarian stimulation methods. However, current IVM protocols lack standardization and often produce lower-quality oocytes compared to those naturally matured in the female body. To address this challenge, innovative biomaterials, particularly hydrogels, offer distinct advantages in cell culture. They provide a three-dimensional cellular environment and enable easy adjustment and characterization of mechanical properties, such as stiffness. In this context, an innovative and reusable bilayer hydrogel system has been introduced to accurately replicate the mechanical properties of the microenvironment surrounding oocyte maturation. This innovative system consists of an outer layer made from either a 3D-printed synthetic polymer (2-vinyl-4,6-diamino-1,3,5-triazine) or a natural polymer (chitosan), paired with an inner layer composed of alginate. By faithfully mimicking the mechanical properties of native tissue within a 3D culture environment, this system significantly improves the quality and developmental potential of oocytes, leading to successful embryo development. It represents a significant advancement in assisted reproductive technologies by addressing the issues of non-standardized IVM protocols and the production of lower-quality oocytes. This innovation has the potential to revolutionize the field and improve the outcomes of assisted reproductive procedures.

### Surface-enhanced Raman Spectroscopy and Artificial Intelligence in Biomedical Research

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#### Abstract

Surface Enhanced Raman Spectroscopy (SERS) is a powerful analytical technique that can provide complex and multidimensional spectra of biomolecules. Due to its sensitivity and low detection limit, SERS is especially useful in the bioanalytical and medical fields, for the detection of disease markers, proteins and other relevant (bio)molecules. However, interpreting of SERS data can be challenging especially in the case of real and complex samples, which contain a large number of unwanted background molecules. In this case the Raman signal from all biomolecules is enhanced, leading to peaks overlapping and making the manual spectra interpretation almost impossible. The application of artificial intelligence (AI) algorithms can facilitate the identification of SERS patterns and relationships in the data, which may not be readily apparent to human analysts. This integration of AI with SERS analysis can lead to the development of highly sensitive and specific analytical and diagnostic tools that can be used in various fields, including bioanalysis and medicine. The combination of AI and SERS offers new opportunities for the detection and identification of targeted biomolecules at very low concentrations. In our work, we demonstrated the AI-SERS combination for the detection and identification of proteins and DNA molecules (at picomolar concentrations), which provides possibilities for the early detection of diseases. In addition, we also applied the SERS-AI combination for the monitoring of various biological processes, including non-invasive and non-destructive monitoring of stem cell growth as well as monitoring of bacteria antibiotic resistance development.

## Development of Washable Antifungal Textiles Through Chemical Reaction of Fluconazole and Trichlorotriazine

Juan Henao<sup>1\*</sup>, Marlon Osorio<sup>2</sup>, Cristina Castro<sup>2</sup>, Juan David Puerta<sup>3</sup>, Tonny Naranjo<sup>3</sup> and German Quintana<sup>1</sup>

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<sup>3</sup>Medical and Experimental Mycology Group, Biological Research Corporation, Colombia

### Abstract

Cotton is highly susceptible to the growth of fungi that impair the properties of the textile and can cause disease. Therefore, efforts are currently being made to develop cotton textiles with biological properties by applying antimicrobial compounds. However, these fail to adhere strongly as they do not have a chemical anchor and are washed away when the garment is washed. In this research, we sought to develop a functional textile using Fluconazole (FLZ) as an antifungal agent and Trichlorotriazine (TCT) as an anchoring molecule in order to improve the chemical bonding in the textile and its durability with washing. Three different procedures for textile development were evaluated by varying the order of reaction between cotton, FLZ and TCT. The textiles produced were characterized by Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM) and antifungal tests against *Aspergillus niger*, before and after fifty accelerated washes. The developed textiles present characteristic bands of FLZ and TCT in the FTIR spectrum, and the SEM images showed that the three procedures performed succeeded in modifying the surface morphology of the cotton yarns, before and after the fifty accelerated washes. In the antifungal tests of the textiles, fungicidal effects were obtained in two of the developed procedures and fungistatic in the third one on *A. niger*.

## Formulation of Eugenol Based Wound Healing Gauze Nanocomposites Towards Enhanced Vasculogenesis for the Treatment of Diabetic Wounds

Lakshimipriya Sethuram\* and Natarajan Chandrasekaran

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### Abstract

Diabetes mellitus is an increasingly chronic and execrable disease which has obtained an epidemic proportion worldwide. India carries 25% of a considerable share in the global diabetes burden. Diabetic wounds remain a major health problem and affects approximately 35% of diabetic patients resulting in lower limb amputation with rapid economic costs. Researchers have designed potential products ranging from saline to skin substitutes for treating chronic wounds. However, it is of great clinical significance to deeply explore on topical application of efficient and controlled drug delivery of bioactive nanomaterials for amelioration of effective blood circulation and anti-inflammatory responses to ulcerated wound area. Here, we have formulated a multifunctional 3D nanoscaffold using PDGF impregnated eugenol-based core-sheath nanofibrous scaffolds (CSNs) for treating diabetic wounds in clinical practice. These PDGF/Eugenol/CSNs revealed excellent absorption efficiency, high level of biocompatibility and biodegradability, sustained ability of sequential drug release in wound fluids, acceptable porosity and water uptake and hem compatible in nature. *In vitro* silver ion release kinetics demonstrated that nanofibers possess a sustained mode of drug release over an extended period. PDGF/Eugenol/CSNs showed greater efficacy against *Staphylococcus aureus* and *Pseudomonas aeruginosa*. *In vivo* diabetic excision wound healing models demonstrated an excellent wound healing efficiency of PDGF/Eugenol/CSNs with maximum percentage of wound contraction and wound closure during the 9<sup>th</sup> day in diabetic rats. Hence, PDGF/Eugenol/CSNs could be a promising wound healing therapeutics and drug delivery platform for efficient transformation in the healing of diabetic foot ulcers.



## Formulation and Performance of Bioactive Hydrogel Scaffold Carrying Chlorhexidine and Bone Morphogenetic Protein

Dongyang Zhou<sup>1,2\*</sup>, Lidi Cheng<sup>1,2</sup>, Dian Xu<sup>1,2</sup>, Zexian Xu<sup>1,2</sup>, Ming Sun<sup>1,2</sup> and Liqiang Chen<sup>1,2</sup>

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<sup>2</sup>School of Stomatology of Qingdao University, China

### Abstract

Infected bone abnormalities are a difficult clinical problem to cure. In this study, a chitosan/sodium alginate temperature-sensitive hydrogel scaffold (CHX@BMP-2-TH) was developed and described with chlorhexidine/ $\beta$ -cyclodextrin (CHX/ $\beta$ -CD) and chitosan/bone morphogenetic protein (CS/BMP-2). The results revealed that adding CHX/ $\beta$ -CD and CS/BMP-2 to the hydrogel improved the mechanical properties and reduced the internal porosity; CHX@BMP-2-TH stimulated MC3T3-E1 osteogenesis and inhibited *Escherichia coli* and *Staphylococcus aureus* growth. CHX@BMP-2-TH is a unique bioactive substance that could be used to treat infectious bone abnormalities.

## Symposium III: Future Materials for Energy, Environment and Sustainability Featured Presentations

### Green Hydrogen and Innovative Materials for a Sustainable Future

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### Abstract

The green hydrogen revolution is gaining momentum as the world seeks to reduce greenhouse gas emissions and combat climate change. This transition from traditional fossil fuels to renewable energy sources like hydrogen is driven by the need to decarbonize the economy. Hydrogen plays a critical role as a feedstock in numerous industries. For example, it is a vital component for producing ammonia, which is essential in fertilizers. Additionally, it is utilized in refining crude oil, manufacturing methanol, and creating a variety of chemicals.

The green hydrogen revolution involves the development of new technologies for the production, storage, distribution, and utilization of hydrogen. There are several options for producing green hydrogen, including electrolysis, biomass conversion, and thermal processes. The use of renewable energy sources, such as solar or wind power, to power these processes makes green hydrogen a clean and sustainable fuel option. While the potential benefits of green hydrogen are significant, there are also challenges to overcome. One of the biggest challenges is the cost of producing green hydrogen, which is currently higher than grey hydrogen and other fossil fuels. Additionally, there is a lack of infrastructure for the storage and distribution of hydrogen, which needs to be developed to enable the widespread adoption of this technology.

The green hydrogen revolution is an emerging technology with enormous potential to transform the energy sector and combat climate change. While there are challenges to overcome, the prospects for this technology are promising, and investment in research and development will be critical in bringing down the costs and scaling up production to enable widespread adoption.

Our work is focused on a comprehensive research and development agenda, spanning from laboratory experimentation to market implementation, with the goal of advancing emerging technologies and demonstrating the viability of existing options. One area of particular interest is the development of innovative materials aimed at promoting the growth of a green hydrogen economy.

## Accurate Characterization of Thermal Radiative Properties for Solar Energy Materials

J. Gabirondo-López<sup>1</sup>, M. Sainz-Menchón<sup>1</sup>, I. González de Arrieta<sup>1</sup>, T. Echániz<sup>2</sup>, I. López-Ferreño<sup>3</sup>, R. Fuente<sup>2</sup>, J.M. Igartua<sup>1</sup> and G.A. López<sup>1\*</sup>

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<sup>3</sup>Applied Mathematics, Faculty of Engineering Vitoria-Gasteiz, University of the Basque Country UPV/EHU, Spain

### Abstract

A key aspect of solar energy research is the development of materials with optimized optical properties in a wide spectral range, from the ultraviolet to the infrared. These optical properties will not only determine the efficiency of solar absorption, but also how heat transfer takes place within the system. The importance of emissivity characterization has been traditionally recognized for solar thermal energy applications, which rely on solar absorbers. However, these characterizations have been usually made at room temperature and in the normal direction. Moreover, hardly any data exists for the emissivity of solar cells.

In this contribution, we present experimental results corresponding to different types of solar absorbing materials. First, we evaluate the optical response of two W-base multilayer coatings for vacuum parabolic troughs, showing their divergent directional response and significantly different total hemispherical emissivities. Secondly, we present results corresponding to black coatings, based on nanoparticles and nanoneedles, intended for application in solar towers in air. Because of the higher solar concentration factor of this technology, preferentially the absorptivity is the parameter that has to be increased. Finally, we demonstrate the capability of our method to measure emissivities close to room temperature by providing results on solar cells with different architectures and analyzing how their directional response differs.

## Hybrid Materials Based on Conjugated Porous Polymers and Covalent Organic Frameworks for Artificial Photosynthesis

Marta Liras<sup>\*</sup>, Mariam Barawi, Teresa Naranjo, Miguel Gómez Mendoza, Laura Collado, Miguel Garcia Teceador, Hakan Bildirir, Freddy Oropeza, Sandra Palenzuela Rebella, Tania Mazuelo and Victor A. de la Peña

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### Abstract

Solar energy conversion plays an important role in the transition to more sustainable energy technologies. Both demographic growth and industrialization leads to an increase in the consumption of solid fuels which the consequent planet temperature rise and appearance of associated environmental problems. Thus, the development of new technologies to storage renewables energy is a matter of importance in the transition to a greener energy pool. In this sense, artificial photosynthesis (AP), which convert CO<sub>2</sub>, and water as raw materials by the action of solar energy in valued chemicals or fuels, could be an attractive solution. Here, the look for new materials able to produce solar fuels as efficient manner is a challenge. Conjugated (micro)porous polymers (CMPs or CPPs) as well as their crystalline analogs Covalent Organic Framework (COFs) have appeared recently as alternative to inorganic semiconductor, metal oxides and chalcogenides, the typical photocatalyst used in AP.

In this talk, I am going to show our last result in the use of CPPs and COFs as well as hybrid thereof in AP processes such as hydrogen production from water and CO<sub>2</sub> photoreduction.

## Static and Dynamic Models of Electrode Coatings in Solid-state Lithium Anode Batteries with Superionic Conductors: Development of a Specifically Tailored Reactive Force Field for Multiscale Simulations

Maddalena D'Amore<sup>1\*</sup>, Moon Y. Yang<sup>2</sup>, Minho Kim<sup>2</sup>, Anna M. Ferrari<sup>1</sup>, Mauro F. Sgroi<sup>1</sup>, Alessandro Fortunelli<sup>3</sup> and William A. Goddard III<sup>2</sup>

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## Abstract

In order to dramatically improve battery performance, it is important to switch from current generation Lithium (Li)-ion batteries (LIB) to next generation Li-metal anodes (LMA). This requires new electrolytes stable against a LMA or else a protective layer to stabilize the solid-electrolyte interface. We are studying most promising Li superionic conductor electrolytes, particularly Argyrodites that belong to the “sulphides family”. Unfortunately, these electrolytes can react with Li anodes therefore, we are investigating how to stabilize solid electrolytes at the interface with the Li electrodes. In particular, we are simulating coatings that decrease degradation with the electrolyte while maintaining high Li<sup>+</sup> conductivity. In the present study, we investigated Li<sub>2</sub>S as possible coating in Argyrodite/Li interfaces. The modelling of chemical and transport phenomena in these systems requires molecular dynamics to be run for  $t \geq 1$  nanosecond on realistic models with  $> 100,000$  atoms, which is far too large for quantum mechanics calculations. Instead, we use the ReaxFF reactive force field, for which reactive molecular dynamics on  $> 100,000$  atoms for  $t > 10$  nanoseconds is practical. To optimize the ReaxFF parameters for a Li<sub>2</sub>S coating on the Li anode we used density functional theory at the level of at PBE0/TZVP and M062X/TZVP level for model systems. We will report the ReaxFF predictions for multiscale reactive simulations on the interfaces.

## Advanced Materials for Tracer-based Sorting to Improve Recyclability of Thermoplastics

Florian Part<sup>1\*</sup>, Christoph Olscher<sup>1</sup>, Aleksander Jandric<sup>1</sup>, Christian Zafiu<sup>1</sup>, Christoph Lechner<sup>2</sup> and Robert Lielacher<sup>2</sup>

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<sup>2</sup>Polymerwerkstatt GmbH, Dr.- Franz – Wilhelm – Straße 2, Austria

## Abstract

Engineering plastics, such as acrylonitrile butadiene styrene or polyoxymethylene (POM), are tailored through compounding to fulfill the technical requirements of e.g. electric and electronic equipment. At the end of their life, these polymers are usually incinerated because they contain additives and fillers that make them difficult to recycle, especially when the waste plastics end up in mixed waste electrical and electronic streams.

Therefore, our research focused on the so-called tracer-based sorting (TBS) concept, whereby marker materials are incorporated into the polymer matrix to facilitate the traceability during sorting processes. We have developed a method to select advanced materials that are safe and recyclable, as their unique optical or spectroscopic fingerprints allow to clearly detect the marked plastics using NIR-, UV-VIS-, or XRF-based detection techniques. Our approach allowed to select three different advanced materials (out of 80 candidates), which were used to produce master batches of marked POM at pilot scale. The selected ‘advanced markers’, which consisted of rare earth elements, were detectable in POM at concentration ranges between 1 and 1000 ppm using XRF. Our case study shows the feasibility of the TBS concept in order to enhance the circularity of engineered plastics.

## New Concepts for the Fabrication of More Efficient and Durable VO<sub>2</sub>-based Smart Glazing

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## Abstract

Vanadium dioxide ( $\text{VO}_2$ ) is one of the most extensively studied materials over the last decade, mainly because it undergoes a reversible phase transformation, which is thermally induced at temperatures  $\sim 68^\circ\text{C}$ , between monoclinic  $\text{VO}_2(\text{M})$  and rutile  $\text{VO}_2(\text{R})$  during heating, leading to drastic changes in optical and electrical properties. This phenomenon makes vanadium dioxide the best candidate for application in so-called “smart glazing”, allowing to block the transmittance of solar energy in the infrared range (heating) without reducing the passage of visible light (illumination). However, the complexity and/or high cost associated with the fabrication processes of  $\text{VO}_2$ -based nanostructures, which is closely related to the complex chemistry of vanadium and its large number of stable oxidation states, have limited the transfer of this technology to the industrial scale. Thus, the development of simple, environmentally friendly, and economically advantageous methodologies for the fabrication of energy-efficient  $\text{VO}_2$ -based surfaces is of paramount importance. Aware of this need, this work proposes alternative and scalable strategies for the synthesis and doping of  $\text{VO}_2(\text{M1})$ -based thin films, which comprise the co-deposition, by magnetron sputtering combined with reactive gas pulsed processes, of  $\text{VO}_x\text{-WO}_x$  thin films on glass substrates in grazing angle geometry (GLAD), and their subsequent controlled and instantaneous oxidation in air atmosphere at high temperature. The exhaustive control of the deposition (layer thickness, composition) and annealing parameters (reaction temperatures and times), together with the superior reactivity with oxygen of high surface-to-volume porous V-GLAD nanostructures, allow the modulation of the properties of such coatings for an optimal solar energy utilization.

## Cellulose Nanocrystal-based Sustainable Inks for Packaging

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## Abstract

Natural photonic structures, such as the helicoidal arrangement of cellulose found in *Pollicia condensata* fruit, are responsible for some of the most spectacular colors in the natural world. Studying these structures provides insight into how biological materials, like cellulose and chitin, can be used to create sustainable colorants.

Cellulose, a sugar-based polymer found in almost all plants, can be extracted from natural sources as cellulose nanocrystals (CNCs) - thin, rigid rods that are less than a micron in length. When CNCs are brought together, they can self-assemble into photonic structures that exhibit brilliant colors under specific conditions.

The intense color of CNC films is due to the helicoidal structure created by self-assembly. By altering the pitch, or the distance between the repeating pattern of the twisted configuration of CNCs, the color of the film can be changed. A larger pitch reflects longer-wavelengths resulting in a red-shifted color, while a smaller pitch reflects shorter-wavelengths, causing a blue-shift. By adjusting the conditions of CNC self-assembly, the visual appearance and color of the films can be controlled.

The objective of this work is to create new pigment-less cellulose-based inks using CNCs, a biopolymer that is fully bio-sourced, biodegradable, and recyclable, and compatible with conventional printing setups.

## Zr-based Metal Organic Framework Loaded with Highly Dispersed Small Size Ni Nanoparticles for $\text{CO}_2$ Methanation

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## Abstract

The conversion of CO<sub>2</sub> to value-added fuels and chemicals is a promising way for CO<sub>2</sub> utilization. The thermal catalytic CO<sub>2</sub> hydrogenation is potential for industrial application and thus received increasing research interest. The chemical sequestration of CO<sub>2</sub> in porous materials is attracting increasing attention as an efficient strategy for the conversion of CO<sub>2</sub> through hydrogenation protocols, due to their large surface area, abundant metal sites, functional organic linkers, and highly ordered porous structure. In this work, we explored the Zr-based MOF (metal organic framework)-545 for CO<sub>2</sub> methanation. Here, we use Operando DRIFT spectroscopy to follow the changes of MOF under CO<sub>2</sub> hydrogenation conditions, temperature up to 300 °C under CO<sub>2</sub>/H<sub>2</sub> (3:1), and pressure (10 bar) in flow reactor conditions. Interestingly, we identify clear elimination of the bridging μ<sub>3</sub>-OH groups of the MOF upon catalysis, while the Zr-based oxoclusters are also strongly modified upon the production of methane. The post-catalytic characterizations (PXRD, XPS, TEM, and EDX-chemical mapping) together with the above *in-situ* FTIR observations allow us to draw a portrait of the transformed MOF-545 as being the active support for CO<sub>2</sub> hydrogenation. We prepared a series of Ni@MOF composites using the Zr-based MOF-545 as a support for catalytic Ni<sup>0</sup> NPs using free-base or Cu metallated porphyrin linkers. The chosen Zr-based MOF-545 support allows not only a high dispersion of small Ni<sup>0</sup> NP due to its adapted porosity, but also permits enhanced cooperation between the highly dispersed Ni nanoparticles and Zr-oxoclusters. We believe that this fundamental work will be applicable to the many unexplored Zr-based MOFs as active support to develop new and highly efficient CO<sub>2</sub> methanation catalysts.

## Electrochemically Prepared Nanopillar Cuprous Oxide Photoactive Layer

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## Abstract

p-Copper oxide (Cu<sub>2</sub>O) has received renewed attention as a promising candidate as the light-absorbing layer for the top cell for silicon solar cells, which can significantly increase the overall theoretical power conversion efficiency, as the 2.1 eV photoactive layer can provide a complementary absorption region of light wavelengths below 500 nm. This research presents a novel electrochemical fabrication method of vertical Cu<sub>2</sub>O nanopillars with lengths in the micrometer order. The Cu<sub>2</sub>O layer was firstly electrodeposited on <111>-oriented Au substrate, from an aqueous solution containing Cu ions, then anodized under 10 V with varying anodizing time. The nanopillar layer was evaluated with UV-Vis, FE-SEM observation, XRD, and XPS measurements. Under the given pH of the anodizing solution, the Pourbaix diagram provided thermodynamic expectations that the Cu<sub>2</sub>O would finally be exposed to conditions in which dissolvable Cu species was most stable. But due to the <111>-preferred oriented Cu<sub>2</sub>O heteroepitaxial electrodeposition and high voltage, grain boundary-etching preferentially occurred, leaving large grains of <111>-Cu<sub>2</sub>O, resulting in the final formation of vertical Cu<sub>2</sub>O nanopillars. Not limited to Cu<sub>2</sub>O, the method can be applied to general oxides or compounds in which grain growth can be controlled, such as electrochemically prepared ZnO, opening a new door for the low-cost electrochemical introduction of large-surface-area nanostructures to photoactive applications.

## Application of High-strength, High-density, Isotropic Si/C Composites in Commercial Lithium-ion Batteries

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## Abstract

Although nanostructured silicon (Si) can overcome the huge volume expansion during lithiation without breakage, in practical applications, it is silicon/carbon (Si/C) composites that are used as anode in lithium (Li) batteries, in which volume expansion of Si can easily transmit to Si/C leading to rupture of composites, therefore, electrical contact loss and poor cyclability. So far, few reported Si/C composites can meet real application requirements. High structural strength of Si/C is a prerequisite for applications and, although it cannot inhibit the expansion when Si becomes Li<sub>15</sub>Si<sub>4</sub>, it can inhibit the irreversible expansion caused by the randomly increase of defect during the repeated phase transition of Si, and can prevent the rupture of composite particles during the compaction and cycling. In this work, a high-strength, high-density, isotropic Si/C composite was applied in commercial cylindrical cells with NCM811, and it exhibited a capacity retention of 83.8% over 1000 cycles at 2.5 - 4.2V and 89.0% at 2.75 - 4.15V, where charge/discharge rate was 0.5C/1C.

## Strategies to Accelerate the Design, Discovery, Development, and Deployment of Materials in the Era of the Digital Transformation

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## Abstract

Traditional approaches to deploy new structural alloys require development cycles that can easily take a decade and are associated with significant economic risks. This is incompatible with current challenges such as global warming, scarcity of raw materials and rising energy costs, which are forcing humankind to rapidly develop sustainable solutions if the level of prosperity of future generations is to be, at least, maintained. To this purpose, innovative and efficient materials solutions along the entire value chain are an essential key. In this presentation, we will show how the digital transformation is enabling the acceleration of the design, discovery, development, and deployment of new alloys for the transportation industry (land, air, and space).

The combination of artificial intelligence, robotic-based labs, high-throughput data generation/analysis, materials combinatorics, predictive simulations, collaborative virtual environments and multi-scale time-resolved experiments result in a suite of data-centric tools whose capabilities will be highlighted through specific use cases: the design of recycled-based alloys, the autonomous testing of metallic structures, the operando study of materials during 3D printing, and the rapid analysis of large experimental datasets. The overall aim is to demonstrate the transformative potential of data-centric approaches to shorten materials development cycles across a range of industrial sectors.

## An Experimental Study on Measurement of Tensile Strength for Envelope Material FV1160 and Structural Strength for Airship Envelope

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## Abstract

In the design of the stratospheric airship, it is necessary to estimate the structural strength of the airship envelop

since it decides the maximum range of the differential pressure and affects the safety of the flight. In this study, three different types of experiments were carried out and results were compared. Firstly, the uniaxial tensile tests were conducted to obtain the uniaxial tensile strength and the relationship between tensile strength and loading speed. After that, biaxial tensile tests were carried out to obtain the biaxial tensile strength. Finally, an exploding test was conducted to test the structural strength of the airship envelop. The value of the structural strength (718.47 N/cm) obtained from the airship envelope exploding test is similar to the value of the biaxial tensile strength (721.38 N/cm) from the biaxial tensile test at low loading velocity and it is only about 69.37% of that (1035 N/cm) from the uniaxial tensile test at the tensile rate of 2 mm/min. This study will support the experimental study on the structural strength and security analysis for airship envelopes.

## Grain Boundary Phenomena in High Entropy Alloys

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### Abstract

The wetting, prewetting, premelting grain boundary phase transitions in the high entropy alloys (HEAs) are analyzed. HEAs are also known as also multicomponent alloys without principal components. The grain boundaries (GBs) in HEAs can be wetted not only by the melt but also by the second solid phase. GB wetting can be complete or partial. In the former case, the second phase forms the continuous layers between the matrix grains and completely separates them. In the latter case of partial GB wetting, the second phase forms the chain of droplets (or particles) in GBs, with certain non-zero contact angles. The GB wetting by the melt can be observed in HEAs produced by all solidification-based technologies. The GB wetting by the second solid phase appears in HEAs after long annealing below the solidus temperature. GB wetting leads to the appearance of novel GB tie lines  $T_{wmin}$  and  $T_{wmax}$  in the multicomponent HEA phase diagrams. The so-called grain-boundary engineering of HEAs permits the use of GB wetting to improve the HEAs' properties.

## Synthesis, Characterization and Crystal Structure of New Bis[hexakis(N-methylimidazole) Zinc(II)] Nitrate Complex for Dye-sensitized Solar Cells (DSSCs) Application

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### Abstract

Dye-sensitized solar cells (DSSCs) have sparked significant scientific attention due to their appealing benefits. With its conjugated electrons, the dye molecule is essential in DSSC materials. The Ru complex is an excellent example of a commercially feasible dye that possesses all of the requisite properties for DSSC use. The recent introduction of low-cost dyes has accelerated the commercialization of DSSCs. Because of their exceptional light-emitting properties, zinc complexes have received a great deal of attention in recent years. Inspired by this, a novel bis[hexakis(N-methylimidazole)zinc(II)]nitrate complex with the formula  $[Zn(C_4H_6N_2)_6]_2NO_3$  was successfully synthesized and determined using X-ray single crystal diffraction analysis, FTIR, UV-Vis and photoluminescence spectroscopy with the intention of being used in DSSC applications. The zinc(II) nitrate complex was found to crystallize in a trigonal crystal structure in the space group P-3, with (a = 19.1227(10) Å, b = 19.1227(10) Å, c = 7.4770(5) Å,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 120^\circ$ , V = 2367.9 Å<sup>3</sup>). The crystal structure of the complex is built up of two discrete monomeric molecules of  $[Zn(Melm)_6]_2^+$  (Melm is N-methylimidazole) cations and nitrate anions. The Zn-N bond lengths were found to be 2.182(2), 2.177(2), and 2.179(2) Å, whereas the N-O bond angles of nitrate ions were situated at distances of

1.202(5), 1.209(4) and 1.234(5) Å. The UV-Vis absorption bands of the complex exhibited two peaks at maximum wavelengths of 215 and 230 nm, corresponding to electron  $\pi$ - $\pi^*$  transitions of the imidazole moiety. Additionally, the complex exhibited blue photoluminescence at 411 nm in the solid state. Furthermore, ongoing stability tests and density functional theory calculations are in progress, and once these are completed, the complex will be evaluated for its suitability in DSSC applications.

## Recent Advances in Spectrally Selective Coatings for High Temperature Solar Thermal Applications

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### Abstract

Solar radiation is an abundant clean source of renewable energy. One of the easiest ways to harness the solar energy is via solar thermal, in which the solar radiation is converted into thermal energy and subsequently to electrical energy by solar collectors. For generating electricity, the collectors require highly specialized surfaces with very high absorptance in the solar spectrum region (that is, 0.3 - 2.5  $\mu\text{m}$ ) and low thermal emittance in the infrared region (2.5 - 50  $\mu\text{m}$ ), known as spectrally selective coatings. One of the main requirements of spectrally selective coatings for high temperature applications is their high temperature stability ( $\geq 400$  °C). Spectrally selective surfaces are the most important component of the concentrated solar power generation technology. Therefore, it is very important to develop and design spectrally selective coatings with high temperature stability. Towards this, the research on nanostructured transition metal nitrides, oxides and carbides has gained a lot of importance in recent years for solar thermal applications. In the literature most of these nitrides and oxides have been prepared using vacuum-based processes which are capital intensive. Accordingly, efforts are currently underway to develop the processes which are cost effective as well as eco-friendly. This talk will present an overview of various high-temperature spectrally selective coatings for solar thermal applications. It will also address the use of new generation 1D and 2D materials which are less explored in the literature. Finally, the presentation will cover the service life prediction of these high temperature solar absorber coatings mainly for power generation applications.

## Calculation Accuracy Improvement of Magnetic Hysteresis Based on Simplified LLG Equation for Electric Machines

Yoshiki Hane\* and Kenji Nakamura

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### Abstract

In recent years, it is strongly desired to develop more efficient electric machines, including power transformers and electric motors, from the viewpoint of energy saving and environmental conservation. Hence, it is necessary to establish an accurate estimation method of iron loss including magnetic hysteresis behavior. The Landau-Lifshitz-Gilbert (LLG) equation, which is one of the representative physical hysteresis models, seems to be one of the practical solutions because its calculation accuracy is considerably high. Although it is generally extremely difficult in practice to analyze magnetic devices of the size of electric machines in terms of computation time and computer capacity, some assumptions for simplification were incorporated into the LLG equation in the previous study, such as not directly considering the effects of domain wall motion. In this way, it is possible to accurately calculate the hysteresis loops and iron losses of electric machines with practical calculation time and cost. In this presentation, we present the several methods for further calculation accuracy improvement of this simplified LLG equation.

## Development of a Radon Adsorption Material Based on Activated Carbon Modified by Potassium Hydroxide

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### Abstract

Radon is the second major factor of lung cancer after smoking. Activated carbon is currently the only commercial radon adsorbing material. To solve the disadvantages of existing radon adsorbing materials modified from activated carbon, these are high cost, no regeneration in the air, and low efficiency of radon adsorbing. Potassium hydroxide modified activated carbon (KAC) was prepared by high temperature roasting. Its adsorption capacity was measured, and its morphology and structure were characterized. The results show that the radon adsorption coefficient of KAC reached  $6.50 \pm 0.13$  m<sup>3</sup>/kg at room temperature (25 °C) and atmospheric pressure (1 bar), which was nearly 50% higher than that of activated carbon. KAC can be recycled in the air, and its radon adsorption performance remains unchanged. The increase of micropore volume of about 0.55 nm is the main reason for the improvement of radon adsorption performance of KAC. It is a kind of radon adsorbing material with strong performance, low cost and convenient regeneration, and it has very attractive prospects.

## New Perspectives on the Li, Na, and K Electrochemical Storage in Hard Carbon

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### Abstract

Our work focuses on understanding Li, Na, and K storage mechanisms in hard carbon electrodes for battery applications. We used density functional theory to evaluate the formation enthalpies of various model systems, calculating the respective voltage profiles and reaction mechanisms. Highlighting the similarities and differences between the alkali ions, we deconvolute all the storage site contributions to the voltage profiles putting forward a unified reaction mechanism. The reaction initiates at edges, defects, and vacancies via adsorption in various energies, giving rise to the initial part of the sloping voltage profile. Intercalation in defective graphene bilayers takes over, representing a solid solution reaction concluding in a voltage plateau dominated by nanopore filling. All alkali metals follow this mechanism once we carefully examine the “hidden” Li voltage plateau. Our electrochemical experiments accurately measure the potential differences matching the calculated behavior for all three alkali ions. The newly gained insights have the potential to significantly advance the optimization of battery performance by aiding in the design of more effective hard carbon electrodes providing clear directions for nanopore size upon synthesis.

## Affordable Measurement of Heat Capacity and Thermal Conductivity of Composites

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### Abstract

Composites are commonly used for energy harvesting applications. When these systems involve heat transfer, measurement of the thermal properties of the polymer components is very crucial. Although well-established

experimental methods for thermal measurements exist, they may not be affordable for all laboratories.

This research work offers a low-cost alternative that has proven to be reliable for making accurate thermal measurements of polymer films. It proposes an experimental set-up that determines both thermal conductivity and thermal capacity with the same test, but in two different regimes. The set-up consists of a succession of layers including copper plates, heat sinks, heat sources, sensors, and insulation layers. A thermal flux is applied and a constant temperature difference to a known thickness of a sample is known. The test operates in a steady state to determine thermal conductivity and in a transient state to determine thermal capacity by determining the time constant. For the same sample, the tests are performed with different heat flows and temperature gradients to ensure that the thermal conductivity and capacity are independent of the experimental conditions.

The study reports measurements for composite (PU/PZT) and polymer (PEDOT:PSS) samples. The results show good agreement with values obtained using established methods.

## Future Materials for Clean Energy Generating Light Water Reactors

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### Abstract

Most nations in the Globe are engaged in decarbonization efforts of the environment. For this purpose, the use of all carbon-free clean energy sources are part of the solution. One of the most important sources of clean energy is nuclear energy since it is weather-independent, and it can produce electricity continuously the 365 days of the year. In the last thirty years in the USA only a couple of newer power-generating light water reactors were connected to the civilian grid. Therefore, there is an effort to avoid the decommissioning of the currently existing 90+ reactors in the country so they can keep contributing to their share of clean energy. One way of extending the life of the current reactors is to retrofit them with advanced materials that will make them more economically and safer to operate. These newer materials for the fuel of the reactors are called Accident Tolerant Fuels or Advanced Technology Fuels. The presentation will include a description of the advantages and detriments of the newer materials compared to the currently used fuel, which is based on the architecture of uranium dioxide fuel pellets encased in slender tubes of zirconium-based alloys.

## High-temperature Thermal Transport Processes and Materials for Solar-thermal Energy Conversion and Storage

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### Abstract

High temperature thermal transport processes and materials are important for the next-generation solar-thermal systems, including concentrating solar power, solar thermochemical fuel production, and thermal energy storage. However, characterizing high-temperature thermal transport is challenging, especially on the corrosive heat transfer media such as molten salt and flowing particles. Additionally, there is a need for materials that are stable at high temperatures and can provide desirable optical, thermal, and thermochemical functionalities. In this talk, we will present our recent work on these two fronts. First, we have developed a non-contact high-temperature thermal transport characterization technique named “modulated photothermal radiometry” (MPR), which can accurately measure thermal conductivity of molten salts and granular media, in both the static and flowing states, at high temperature. In particular, the MPR measurements on flowing ceramic particles reveal that thermal transport is substantially altered compared to their static counterparts. This has a major impact on the design of particle heat exchangers. Second, we have developed high-temperature stable high-entropy oxides, which can be used to



coat ceramic particles to enhance their optical and thermal properties, thus showing promises as multi-functional materials for next-generation solar-thermal systems.

## Effect of Oxygen Content in Cathodic Copper on the Ductility of Copper Wires

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### Abstract

The concentration of impurities on cathodic copper affects the mechanical properties, i.e., ductility, of the derived copper wires. The results of standard mechanical test to evaluate ductility show that there is not a conclusive correlation between the impurities content in the cathodes and the ductility of copper wires. In this work, from traction tests on copper wires and observation of their fracture surfaces by means of scanning electron microscopy and energy dispersive X-ray spectroscopy, it has been concluded that the principal impurity affecting the ductility of copper wires is oxygen, mainly incorporated during the melting of the cathodes and the casting of the rods. Also, to discriminate the effect of oxygen content in copper ductility, the used probes must not be annealed, since in this case O in the form of cuprous oxide particles is mainly segregated at grain boundaries manifesting his deleterious effects and diminishing the ductility. On the contrary, if the probes are annealed the Cu<sub>2</sub>O particles are more dispersed on the matrix, with minor negative effect on the ductility, and this behavior is independent for oxygen up to 650 ppm on the rods.

## Performance and Opportunities of an Air-to-PCM Heat Exchanger in Buildings

Peter van den Engel<sup>1\*</sup> and Michael Malin<sup>2</sup>, Nikhilesh Kodur Venkatesha<sup>1</sup> and Luigi Antonio de Araujo Passos<sup>1</sup>

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### Abstract

In addition to air-to-air or air-to-water heat exchangers in air handling units, an air-to-PCM-battery of calcium chloride hexahydrate is a favourable extra option. This makes it possible to store most of the heat not gained by the mass of the building or heat exchanger in the air handling unit. Storing of cold from outside air during the night in the cooling period will reduce the cooling demand as well. Detailed measurements and simulations of PCM in CFD and MATLAB have been executed. The PCM is stored in a battery integrated in a climate tower of the transparent Co Creation Centre at the TU-Delft. The energy performance of this building over a year has been predicted with DesignBuilder and in MATLAB. In MATLAB a very detailed model of the building with all the components has been developed in which Model Predictive Control is integrated, making it possible to optimize the energy consumption. The MATLAB-model showed that by a combination of passive and active control strategies with PCM, a heat exchanger and outside sunshade the energy consumption can be reduced with more than 50%. Measurements are still executed and compared with the outcome of two different digital twin programs, MATLAB and Priva ecoBuilding. Both programs can control and optimize the BMS-system. One of the conclusions is that only digital twins cannot solve all the control-errors and that logical human assessment is always necessary, especially during the first period of use.

## Synthesis, Characterization, Conformational Switching, and Photophysical Properties of BODIPY-Fullerene Resorcin[4]arene Cavitand

Selina X Yao<sup>1</sup>, Yuguang Sui<sup>2</sup> and Hai Xu<sup>2\*</sup>

<sup>1</sup>*Rivian Automotives, United States*

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## Abstract

Chlorophyll is a temperature- and pH-sensitive pigment responsible for the absorption of light in photosynthesis, which ultimately provides energy for the process. The inhibition of photosynthesis and energy transfer can occur due to a decrease in temperature or pH levels. To imitate this process, two new donor-acceptor dyads, R-BF-Cl and R-BF, with bridging the donor BODIPY and the acceptor fullerene by resorcin[4]arene cavitand, were synthesized and characterized for light harvesting in artificial photosynthesis. Steady-state absorption spectra showed no interaction between BODIPY and C<sub>60</sub> in R-BF-Cl or R-BF underground state. However, steady and transient state fluorescence emission spectra showed singlet-singlet energy transfer occurring from BODIPY to C<sub>60</sub> in R-BF-Cl or R-BF with the *vase* conformation, with calculated rate constants and efficiencies of  $7.39 \times 10^7 \text{ s}^{-1}$  and 13.05%,  $6.39 \times 10^7 \text{ s}^{-1}$  and 11.48%, respectively. R-BF-Cl undergoes conformational switching from the *vase* to the *kite* under pH induction in CHCl<sub>3</sub> or CHCl<sub>3</sub>/CS<sub>2</sub>, not CD<sub>3</sub>COCD<sub>3</sub>/CS<sub>2</sub>, and the singlet-singlet energy transfer rate constant and efficiency of the *kite* conformation R-BF-Cl are calculated to be  $4.3 \times 10^7 \text{ s}^{-1}$  and 13.24%, respectively. However, no photo-induced energy transfer occurred in R-BF-*kite*. This study successfully developed two stable donor-acceptor dyads, R-BF-Cl and R-BF, for light harvesting in artificial photosynthesis. The findings illustrate the impact of resorcin[4]arene cavitands as bridges on the interaction between the donor and acceptor moieties of artificial photosynthetic reaction centers and demonstrate the energy transfer dynamics through molecular conformations of R-BF-Cl and R-BF, respectively.

## Degradation of Colorants in Water by Employing a Fe-based Metallic Glass

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## Abstract

An iron-based metallic glass (MG) was employed for cleaning contaminated water containing different concentrations of colorants. Specifically, aqueous solutions containing methyl orange and methylene blue were treated employing metallic glass powder and ribbons. The effect of pH, colorant concentration, surface contact area, and temperature on the colorant degradation efficiency was studied here. Discoloration of both contaminated samples was observed as a function of time when in contact with the powdered and melt-spun MG. A higher degradation efficiency was observed when both dyes were in contact with the MG having a larger contact surface, i.e., with the MG in the powdered form. The effect of temperature and agitation on the discoloration efficiency is also reported here. It was demonstrated here that the use of affordable iron-based MGs is promising for the degradation of colorants commonly employed in the textile industry.

## Young Researchers Presentations

### Computational Investigation of $\text{YSr}_2\text{Cu}_2\text{FeO}_{7.56}$ for SOEC Applications

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#### Abstract

The air-electrode materials studied as components of solid oxide fuel cells (SOFCs) are, generally, of potential interest for solid oxide electrolyzers (SOEC) applications. In SOFC the air electrode conducts the oxygen reduction reaction (ORR), while in SOEC the materials act as an anode, catalyzing the oxygen evolution reaction (OER). Cuprates belonging to the  $\text{YSr}_2\text{Cu}_2\text{MO}_{7+\delta}$  (M = Co, Fe) systems have been recently studied as air electrodes for SOFC. Within this oxides family,  $\text{YSr}_2\text{Cu}_2\text{FeO}_{7.56}$  is a p-type semiconductor with  $\text{Fe}^{3+}/\text{Fe}^{4+}$  and  $\text{Cu}^{2+}/\text{Cu}^{3+}$  mixed valence, which exhibits an interesting electrochemical behavior associated with catalytic activity in the ORR. We aim to explore the bifunctional application of  $\text{YSr}_2\text{Cu}_2\text{FeO}_{7.56}$  in both SOEC (anode) and SOFC (cathode). In this contribution, we present a computational study of  $\text{YSr}_2\text{Cu}_2\text{FeO}_{7.5}$ . DFT methods using the SCAN functional correctly reproduce the crystallographic and electronic structures of  $\text{YSr}_2\text{Cu}_2\text{FeO}_{7+\delta}$  ( $0 < \delta < 1$ )<sup>2</sup>. Hence, the SCAN functional is employed to investigate the basic properties of  $\text{YSr}_2\text{Cu}_2\text{FeO}_{7.5}$  in view of SOEC application, such as the oxygen vacancies energetics, the electronic conductivity, and the oxide ion mobility.

#### Acknowledgements

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### Sustainable and Smart Polyethylene Oxide/Sodium Alginate-based Electrospun Nanofibrous Superabsorbent Mats as Controlled Release Fertilizer Systems

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#### Abstract

Meeting agricultural requirements, without significantly affecting the soil-water ecosystem in terms of delivering agrochemicals (urea, NPK) for the growth of plants, has become a thematic challenge, particularly, in view of the increasing population, loss of biodiversity, and contamination of soil-water interfacial ecosystems due to overuse of synthetic agrochemicals. In this regard, the development of microplastics free polymer-based electrospun micro/nanofibrous assemblies will act as a sustainable controlled release fertilizer systems (CRFs) by optimally promoting both agro-output and “precision farming”, without significantly aggravating water/soil pollution. Thus, our research work aims at designing of mechano-functionally engineered NPK-loaded optimized polyethylene oxide (PEO)/sodium alginate (SA)-based electrospun nanofibrous constructs as potential controlled nutrient release substrates with improved and sustainable physico-mechanical performance for agricultural and horticultural practices. The variation in microstructural, morphological, thermal, viscoelastic, and mechanical attributes of NPK loaded PEO/SA blended electrospun mats have been evaluated to systematically establish their structural stability. The rate of biodegradability, swelling properties, water retention capacity and nutrient release behavior in both soil and water media were also investigated to ascertain their emerging potential as CRFs for sustainable agriculture. Further, to validate the effectiveness of mats on plant growth, pot experiment of capsicum (*Capsicum frutescens*) was conducted, and the results revealed that the germination rate, plant height, root length, dry and fresh weight of root, and stem length treated with the electrospun mats were higher than those of treated with the primitive NPK.

## Low Temperature Synthesis of High Entropy and Entropy-stabilized Metal Sulfides and Evaluation in Hydrogen Evolution Electrocatalysis

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### Abstract

High entropy metal chalcogenides are materials containing 5 or more elements in the disordered sub-lattice. These materials exploit a high configurational entropy to stabilise their crystal structure, and have recently become an area of significant interest for renewable energy applications such as electrocatalysis and thermoelectrics. Herein we report the synthesis of bulk particulate HE zinc sulfide analogues containing four, five, and seven metals. This was achieved using a molecular precursor cocktail approach with both transition and main group metal dithiocarbamate complexes which are decomposed simultaneously with a rapid and low-temperature annealing process to yield high entropy and entropy stabilised metal sulfides. These materials were characterised by powder XRD, SEM and TEM analysis, along with EDX from both SEM and STEM. The entropy stabilised (CuAgZnCoMnInGa)S material was also demonstrated to be an excellent electrocatalyst for the hydrogen evolution reaction when combined with conducting carbon black and achieved a low onset overpotential.

## Sulfur Infiltration Study on a Palm Kernel Shell Derived Activated Carbon to Improve the Performance of Li-S Cells

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<sup>2</sup>Faculty of Engineering, Metropolitan Technological Institute -ITM, Colombia

### Abstract

Lithium-sulfur batteries stand out among new candidates for energy storage due to their high theoretical specific capacity (1675 mAhg<sup>-1</sup>). To overcome some drawbacks, the use of carbon substrates as sulfur hosts has been proposed. Lignocellulosic residues have been studied due to lower cost and to give added value products. However, it is necessary to optimize the preparation of the sulfur-carbon composite evaluating aspects such as porosity, inorganic matter content, and sulfur infiltration methodology to obtain a material with optimal conditions to improve the performance of Li-S cells.

In this work, palm kernel shell was used to obtain an activated carbon (AC), focusing its study on sulfur infiltration in relation to the mostly microporous textural properties of the AC. The S/AC composites were prepared at 10:90 ratio with infiltration times of 3 and 6 h. Initially, TGA suggested that short infiltration times would be sufficient to have an appropriate sulfur infiltration inside the porous structure, as opposed to the 12 h widely used in the literature. The composites were evaluated using lithium metal and LiTFSI as anode and electrolyte, respectively. The sample at 6 h has the highest initial discharge capacity, and capacity stabilizes since cycle 15<sup>th</sup> for both samples, moreover, the sample at 3 h has a higher capacity and a lower capacity loss between cycle 25 and 60 (13.5%) compared to the sample with longer infiltration time (26.6%). Nevertheless, AC contains nearly 20 % of inorganic matter, it is expected that removing minerals will increase capacity and stability.

### Acknowledgements

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## Adiabatic Solid-state Hydrogen Storage

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### Abstract

The increase in conventional fuel consumption has led to climate change issues, driving research for alternatives to reduced carbon emissions. Hydrogen is being explored as a sustainable fuel for transportation and industry. However, its low volumetric energy density at atmospheric conditions is a major challenge for its widespread applications. Two mature methods have been developed: compressing gaseous hydrogen to 700 bar or transforming it into a cryogenic liquid. nevertheless, they pose risks and require energy. Solid-state hydrogen storage (SHS) involving solid-gas reactions, provides higher energy density, and potential for fast refueling, offering a promising solution to hydrogen storage challenges. SHS materials, including metal hydrides, complex hydrides, and porous materials, have potential for high hydrogen storage capacities and fast kinetics. However, they often require high operating temperatures. Recent advances have focused on improving their properties through additives, nanoscale engineering, and new synthesis methods. In addition, heat management in SHS improves the storage efficiency, which can be achieved through thermochemical energy storage (TcES). The objective of this research is to explore the potential use of calcium-sulfate and phosphogypsum (PG) as TcES materials in combination with metal hydride for SHS in an adiabatic reactor. Our goal is to develop an affordable and efficient hydrogen storage reactor by utilizing PG as TcES material, widely produced as waste by fertilizer companies worldwide and coupling it with abundant metal hydrides. This study involves analyzing and characterizing the materials, enhancing their properties, and simulating the adiabatic SHS process to explore the potential of this novel approach.

## Functionalised Porous Materials for CO<sub>2</sub> Capture and Conversion

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### Abstract

Economic growth is tied to greenhouse gas (GHG) emissions, particularly carbon dioxide (CO<sub>2</sub>) resulting from fossil fuel combustion. With the atmospheric concentration of CO<sub>2</sub> currently at 421 ppm, it has become the most significant contributor to global GHG emissions. Consequently, there is a need for research and technological advancements in capturing, storing, and converting CO<sub>2</sub>. Promising materials in this field are porous organic polymers, specifically conjugated microporous polymers (CMPs). CMPs possess  $\pi$ -conjugated structures, permanent porosity, as well as thermal and chemical stability. Among CMPs, polytriphenylamine (PTPA) networks represent an intriguing class due to their characteristics, such as redox activity and conductivity. These polymers hold potential for catalytic applications, enabling the capture and conversion of CO<sub>2</sub> into valuable products. Notably, the inclusion of carboxylic acid functional groups demonstrates promise, as they exhibit high binding capabilities with CO<sub>2</sub>. In this study, we present a novel class of carboxylic acid functionalised PTPAs. By changing reaction conditions and implementing post-synthetic modifications, we obtained a series of polymers with moderate surface areas and CO<sub>2</sub> uptake capacities (up to 543 m<sup>2</sup>/g and 15.59 wt.%, respectively). The materials exhibit excellent catalytic efficiency (93% conversion) in CO<sub>2</sub> fixation reactions with epoxides without the need for any additives under mild reaction conditions. Moreover, our preliminary investigations into the electrochemical reduction of CO<sub>2</sub>, utilising these networks, reveal promising electrocatalytic activity.



## Novel Class of Metalorganic Fluorine-free Solutions for the Transient Liquid Assisted Growth of High-performance Superconducting $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ Films

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### Abstract

The unparalleled feature of high temperature superconducting (HTS) materials of lossless electrical current conduction up to liquid nitrogen temperature and at high magnetic fields has encouraged the study of  $\text{REBa}_2\text{Cu}_3\text{O}_7$  (REBCO, RE = rare earth elements) systems to unravel the opportunities towards highly efficient electrical transport and high field magnets applications. The excessive production costs of the commercialized HTS coated conductors are impeding their worldwide spread [1]. Nonetheless, the development of chemical solution deposition (CSD) techniques enabled the manufacturing of high-performance and low-cost nanostructured epitaxial HTS superconductors. Ground-breaking physical properties were initially obtained through the trifluoroacetate metal-organic decomposition (TFA-MOD) route. However, the global plea for greener chemical processes led to the introduction of fluorine-free solutions as precursors for epitaxial  $\text{YBa}_2\text{Cu}_3\text{O}_7$  (YBCO) superconducting films. Coupling these to the high-throughput process Transient Liquid Assisted Growth (TLAG) grants growth rates beyond 1000 nm/s [2]. We developed a novel class of robust fluorine-free solutions compatible with TLAG aiming for high-performance thick films, main requirement for the industrial application of CSD-TLAG. The innovative design of a propionate-based metalorganic solution through facile and low-cost synthetic methods and careful selection of amine additives ensured an important decrease in the overall cost of YBCO fabrication. Impressive thickness of 2.7  $\mu\text{m}$  was obtained in nanocrystalline films of highly homogeneous nature exhibiting extremely low porosity (1 - 2 %), finally resulting in high-performance epitaxial YBCO films [3]. The steps towards the successful advancement of this research will be presented, with special focus on solution rheological characterization (EPR, TGA) and detailed microstructural analysis (TEM).

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## Structure Activity Relationship of $\text{La}_{1-x}\text{Nd}_x\text{CoO}_3$ Nanostructures Toward Oxygen Electrocatalysis

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### Abstract

Rationalizing the activity of transition metal oxides (TMOs) towards reactions such as the oxygen evolution (OER)

and oxygen reduction (ORR) reactions in terms of their composition and crystal structure is one of the grand challenges in electrochemical energy conversion systems. TMO electrocatalysts are a vast family of compounds with a wide range of structural motifs, dimensionalities, and electronic properties, ranging from insulator to metallic conductivity [1, 2]. In this contribution, we will provide a detailed study of the structure and activity of  $\text{La}_{1-x}\text{Nd}_x\text{CoO}_3$  perovskites, with  $x$  ranging from 0 to 1. We will assess parameters such as coordination number, bonding, and oxidation state of Co as a function of  $x$ . OER activity increases as the Nd content in the A-site increases up to approximately 50%. We correlate this trend with evolution of Co d-states as a function of composition as probed by electrochemical measurements and DFT calculations. The electrochemical and computational results are supported by structural analysis obtained from X-ray absorption spectroscopy, X-ray photoelectron spectroscopy, X-ray diffraction, and electron microscopy.

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## Yttrium Doped Hexagonal Boron Nitride (h-BN) Nanomaterial Enhancement for Hydrogen Storage

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### Abstract

The increasing global energy demand and the imperative to mitigate carbon emissions have established green hydrogen as a highly potential substitute for conventional fossil fuels. Green hydrogen is generated by using renewable energy sources, providing it an economically sustainable and environmentally benign form of energy. The objective of solid-state hydrogen storage is to store hydrogen within a solid matrix, providing possible benefits such as enhanced safety and increased energy density compared to conventional storage techniques like compressed gas or liquid hydrogen. Nevertheless, the advancement of solid-state storage materials that are both efficient and economically feasible remains a persistent issue, prompting ongoing research in this domain. Boron nitride (BN) nanocomposites have predominantly been documented in the literature for their application in the storage of molecular hydrogen by chemisorption and physisorption, encompassing a broad spectrum of temperatures and pressures. Various BN nanocomposites have been employed for hydrogen storage, including BN nanotubes, h-BN, p-BN, open-ended BN, and BN clusters. The physisorption process is characterized by a rise in hydrogen adsorption by manipulating surface area, pressure, and temperature reduction. Though the 2D configuration of boron (borophene) is a new material. This material's unique shape and electrical features also enable it to exhibit a larger capacity for hydrogen adsorption compared to complicated hydrides based on metals, thereby exceeding the targets established by the U.S. Department of Energy. The electronic structure and hydrogen storage capability of yttrium-doped BN has been theoretically investigated using first principles density functional theory. The adsorption energy results between Y-BN complex and hydrogen molecules ranged from -0.133 eV to -0.178 eV which is an acceptable range for an ideal  $\text{H}_2$  storage material.

## Concentrating Electron and Activating H-OH Bond of Absorbed Water on Metallic $\text{NiCo}_2\text{S}_4$ Boosting Photocatalytic Hydrogen Evolution

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## **Abstract**

As a metallic cocatalyst, the photothermal effect of NiCo<sub>2</sub>S<sub>4</sub> in the process of photocatalytic hydrogen evolution has not been deeply discussed elsewhere. It has been well known that how to intrinsically speed the photogenerated electrons transfer and active absorbed Water (\*H<sub>2</sub>O) to release more hydrogen proton (\*H) are extremely meaningful to photocatalytic hydrogen evolution improvement. Herein, a convenient and mild two-step solvothermal strategy was developed to meticulously design the interface contact structure between a noble-metal-free cocatalyst NiCo<sub>2</sub>S<sub>4</sub> and semiconductor ZnIn<sub>2</sub>S<sub>4</sub> nanoflower, which facilitated the charge rearrangement at the interface to boost the separation of photogenerated carriers. Importantly, photothermal effect induced by NiCo<sub>2</sub>S<sub>4</sub> was demonstrated to ameliorate slow kinetics of water spilling with the apparent activation energy reduction from 50.5 kJ/mol to 38.8 kJ/mol, which was responsible for improving photocatalytic hydrogen evolution rate of 6834.6 μmol.g<sup>-1</sup>.h<sup>-1</sup> accompanied by apparent quantum efficiency of 13.0% at 400 nm. The electron transfer was accelerated due to localized electric field enhancement determined by finite difference time domain simulations. The decline of Gibbs free energy barrier of adsorbed water from 2.94 eV on ZIS to 1.62 eV on NCS/ZIS resulted in H-OH bond activating was demonstrated using density functional theory. This work will provide an effective pathway to design semiconductor-metal-based photothermal assisted photocatalytic system and expand the application of metallic NiCo<sub>2</sub>S<sub>4</sub> in solar-to-fuel conversion.

## **Symposium IV: Materials for Electronics, Optics and Photonics**

### **Featured Presentations**

#### **Low-power Laser Manufacturing of Circuitry**

**Jose Marques-Hueso\***

*Heriot-Watt University, United Kingdom*

#### **Abstract**

This talk will present a technique that enables the direct light writing of metal tracks on a variety of substrates, including 3D printed materials. The light exposure through direct laser writing facilitates the nucleation of silver nanoparticles on the surface. Later, these nanoparticles are used as nucleation layer for metal plating, which results in conductive copper microtracks. Two different catalytic techniques have been developed to accelerate the patterning photoreactions, a bio-inspired technique, as well as a photography-inspired technique that increases the writing velocity by up to two orders of magnitude. One of the advantages of requiring low power is to be able to use inexpensive equipment, since pulsed lasers can be avoided, which reduced capital costs by two orders of magnitude. Different materials have been studied as substrates, including biodegradable polymers, high temperature plastics and elastomers. The technique provides free-form manufacturing in 3D, with a high throughput and resolution (25 μm). The talk will close with a technique that provides a shortcut for building 3D circuitry from photopolymers, which enables the direct manufacturing of complex parts by 3D printing.

#### **Solution-processed Polyoxometalate-based Memory Materials**

**Kirill Monakhov\***

*Leibniz Institute of Surface Engineering (IOM), Germany*

#### **Abstract**

Polyoxometalates (POMs) have emerged as a highly promising class of molecular memories [1]. POM structures containing vanadium centers as electron charge and spin carriers can be transferred in form of memristive single

particles directly from solution [2] or through the gas phase using electrospray [3] on technologically significant surfaces. For example, Lindqvist-type POM with a redox-active, diamagnetic ( $V_6O_{19}$ ) core stores 2 bits of information for its 4 electrically generated logic states at room temperature and low potentials below 2 volts [4]. Charge-balancing POM cations can mediate electron transfer between POM anions that act as physical multi-state switches [5, 6]. The charge stabilization of POMs on conducting surfaces can be ensured by their supramolecular self-assembly with macrocyclic ligands, such as cyclodextrins [3]. POMs containing vanadium are able to store multiple different, potential-induced logic states at room temperature. An electrical contacting of POM-functionalized heterostructures remains a challenge that opens exciting possibilities for the study of surface-confined POMs in in-memory computing and neuromorphic applications.

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## Localized Plasmon Resonance Biosensing Efficiency Improvement by Different Arrangements of Nanoparticles

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### Abstract

Nanostructures consisting of noble metals show unique optical properties, such as the phenomenon of plasmon resonance, which is based on the collective oscillations of the conduction electrons in the nanoscale confinement. Over the past two decades, advancements in both understanding physical phenomena and fabrication techniques have motivated plasmonic nanostructure research and development. The plasmonic properties of the free-standing individual subwavelength particles with various materials and morphology, such as spheres, cubes, rods, etc., nanoparticle oligomers and their random aggregates have been widely explored. Compared with the individual particles, nanoparticle arrays can produce an even more enhanced optical near field in the nanometer-scale gap between particles acting as subwavelength resonators for surface plasmons. In surface plasmon sensors, the plasmon resonance is sensitive to changes in environmental refractive index induced by adsorption or binding of molecules on the material surface. Ensemble measurements could improve the signal-to-noise ratio, but at the same time, variations would result in a broadening of the integral resonant curve thereby hampering the sensor performance. This interplay is studied. When spotting, often a coffee stain effect, i.e. aggregation of particles along the borderline



between the drop and environment is observed. The effect of the particle aggregations on the collective response of the system and possibilities of increasing the sensing efficiency is studied as well.

## Molecular Design on Semiconductive Polymers for Optoelectronics with High Device Performance: Single Polymer Approach

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### Abstract

Semiconductive polymers possess charges and light interconversion capabilities and are suitable for applications in light emitting diode (LED) and photovoltaic cell (PV) and other semiconductor devices. Upon doping, they become conductive and can be used as anti-static charging material (ASCM). The proposed “single polymer approach” is to integrate various functional moieties (including electroluminescence, electron/hole transports, interfacial dipole, energy level tuning, and shielding triplet energy back transfer, and acid dopant) into conjugated polymers as side chains or chain ends for improving the performances and simplifying the device fabrication process. In PLED, we discovered: sequential energy transfer phenomenon, self-organization of poly(fluorene)s into well aligned beta-phase, effective shielding of triplet energy ( $E_T$ ) back transfer from phosphor dopant to host polymer with lower  $E_T$ , creation of gradient HOMO levels for effective hole injection in spiro-poly(fluorene)s across 1.4 eV to core-shell QD for efficient light emission, single polymer able to emit sharp red-green-blue emissions simultaneously, creating pseudo-metallic state of metal ion by intercalating it into crown ether cavity grafted onto poly(fluorene) as electron injection layer so that high work function metal such as aluminum can be used as cathode. Recently, we proposed  $\sigma$ - $\pi$  conjugated polymers with silicone or germanium as central atom in the polymer backbone to provide higher triplet energy than those of  $\pi$ - $\pi$  conjugated polymers, allowing a use of blue phosphor and thermally activated delayed fluorescent molecules as guest and giving record high external quantum efficiency. In PV, we discovered: electron transport polymer having multiple functionalities as optical spacer, electron transport, and hole blocking; and 2-D low bandgap polymer (PTB7-Th); and block copolymer blended with quantum dot as active layer for lower material cost and promoted device stability. In ASCM, we developed the first water-soluble, environmentally stable self-doped polyaniline with uniform conductivity in molecular level.

## Oligomer Conductors Modelled on the Doped PEDOT Family

Hatsumi Mori\* and Tomoko Fujino

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### Abstract

Environmentally friendly organic electronics, which are highly compatible with humans and made from inexpensive elements, are attracting increasing attention. Currently, polymeric conductors are used as materials for organic electronics, but due to their structural disorder, a sufficient understanding of the conduction mechanism, and precise conductivity control have not yet been achieved, and contributions from condensed matter research are strongly demanded. In this study, we focus on oligomer conductors, which are allocated on the boundary between polymeric conductors, which are practical but difficult to elucidate the conduction mechanism and precisely control their properties, and small-molecule conductors, where the conduction mechanism can be elucidated through research of structure-property correlation, but the application based on films is limited. In oligomer conductors, the advantages and knowledge of both polymers and small molecules can be incorporated. In this presentation, our recent studies related to oligomer conductors modelled on PEDOT family are introduced.



## Characterization of Cu-Sn-In System in Pb-free TLP Bonding

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### Abstract

This work presents the results obtained from experimental and theoretical studies made on the ternary Cu-In-Sn system in the context of Pb-free Transient Liquid Phase Bonding (TLPB) for application in electronics. The TLPB involves melting, dissolution, saturation, reaction (in some cases) and homogenization. This joining technology is used from structural to electronics applications. One goal of TLPB is to get thin joints which can withstand high temperatures and stresses by a proper filler material and manufacturing parameters selection, including dissimilar materials bonding. Since there are still some discrepancies regarding the nature of the Cu-In-Sn intermetallic phases (IP), the phase identification, crystallography, microstructure and phase transformation kinetics during the diffusion-reaction process occurring at the interfaces of Cu/InSn/Cu joints should be deeply understanding in order to get the optimal manufacturing parameters, i.e., filler material composition and thickness, time, temperature, pressure and atmosphere. The results showed the formation of two IP layers, Cu-poor and the Cu-rich, which grow by diffusion and reaction control process, respectively. The Cu-poor layer consists in  $\eta$ -phase (Cu<sub>5</sub>Sn<sub>6</sub>/Cu<sub>2</sub>In) with a duplex morphology of large and small grains. While the Cu-rich layer presents a fine microstructure of a mixture of  $\zeta$ -Cu<sub>10</sub>Sn<sub>3</sub> and Tau-phase (Cu<sub>11</sub>In<sub>2</sub>Sn<sub>4</sub>/Cu<sub>16</sub>In<sub>3</sub>Sn) when the filler material is close to eutectic composition. If the filler Sn content increases, the  $\epsilon$ -Cu<sub>3</sub>Sn appears. While, if filler material Sn content decreases, the  $\delta$ -Cu<sub>7</sub>In<sub>3</sub> forms. The Cu-rich layer is quite attractive because of its fast kinetic, high thermal stability and good mechanical behavior.

Short Biography: In 1998 I graduated in Chemical Engineering at UNCo in Neuquén-Argentina. In 2002 I obtained my PhD in Natural Sciences at University of Stuttgart/Max-Planck-Institute in Stuttgart-Germany. During my post-doc at the IFF-University of Stuttgart/IPA-Fraunhofer Institute (2002-2004), I worked in Surface Engineering. Since 2005, I have been working as a professor in Materials Sciences at UNCo and as a researcher at the CONICET. Since 2016, I am the director of the Institute for Research in Technologies and Engineering Sciences (IITCI CONICET-UNCo).

## Photopolymerizable Luminescent Resin for Dosimetry Nanodevices

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### Abstract

This work presents a functional material that can be 3D printed and used as a molecular dosimeter to measure the amount of vitamin D produced by skin exposure to solar UV radiation for personal monitoring. The photopolymerizable molecular nanocomposite we produced contains an active photonic phase constituted by Eu(btfa)<sub>3</sub>bipy complex and a resin as a polymeric structural passive phase, 3D printed as discs with thicknesses ranging from 50 to 300  $\mu$ m. The Eu<sup>3+</sup> complex guarantees the memory effect through the irreversible quenching of luminescence proportional to the dose, with the sensitivity inversely proportional to the thickness of the printed discs. The photonic signal was transmitted via Bluetooth to a smartphone by a reader we developed to convert the cumulated UVB dose into a cutaneous dose of vitamin D<sub>3</sub>. To validate the devices in the relevant environment, moving the TRL to 7, it was exposed to solar radiation from 9:00 am to 3:00 pm at UV Index 7 (Latitude -8,055, Longitude -34,952). The accumulated UV dose measured 19,2 mJ/cm<sup>2</sup> of UVB, and an estimated average dose of 440,5 IU/h of vitamin D<sub>3</sub> produced by type 3 skin without sunscreen. The calculation used software developed for smartphones by our group using the quenched <sup>5</sup>D<sub>0</sub>-<sup>7</sup>F<sub>2</sub> 615 nm Eu<sup>3+</sup> luminescence as input. A dosimeter with a thickness of 300  $\mu$ m (which has a luminescence quenching of 72% for a dose of 20 J/cm<sup>2</sup>) can be used by the user for an average of 20 days. This device was developed in a SibratecNano project (CNPq/FINEP).

## Towards Large-scale Fabrication of Piezoelectric Thin Films for Stretchable and Wearable Devices

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### Abstract

During the last years, diverse piezoelectric wearable devices have been reported based on well-known rigid ceramics. However, polymers such as polyvinylidene fluoride, and its copolymers, comprise an exciting technology development because of their biocompatibility, stretchability, and high versatility in the fabrication of piezoelectric sensors, actuators, and self-powered wearable devices. Unfortunately, the lack of fabrication processes for large scale and the lower piezoelectric properties of polymers, compared to rigid ceramics, are still halting the full progress and commercialization of such devices. In this work, we propose nozzle-less ultrasonic spray coating as a novel fabrication method for large-scale fabrication of stretchable piezoelectric films with low cost, less restrict by heteromorphic substrate structures, good control of thickness, homogeneity, and reproducibility. Additionally, we add different fillers into the polymer matrix to enhance the piezoelectric, mechanical, or electrical properties of the material. Engineering devices, such as tactile sensors and wearables have been fabricated by the implantation of the fabricated stretchable piezoelectric films showing their potential in the progress of self-powered and health monitoring applications.

## A Room Temperature Approach to Preparing Copper Films with Exceptional Conductivity

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### Abstract

Copper (Cu) has attracted much attention in the electronic industry emerging as a competitive candidate to silver for conductive applications. The main driving force being the high conductivity Cu offers at a significantly low cost. However, full exploitation of the capabilities of Cu is still impeded because of the higher susceptibility to oxidation which retards its long-term conductivity and therefore the stability of resultant devices and technologies. Use of ligands to stabilise Cu is an effective approach to mitigate susceptibility to oxidation, however, this also means that high temperatures are required to decompose any ligands/additives (usually long saturated carbon chains) introduced to the ink formulation to facilitate interaction and fusion of adjacent particles to achieve conductivity. The complete removal of stabilizing agents reduces stability of the resulting film, promoting oxidation. To this end, recently we have successfully developed a simple yet very effective approach to fabricating stable copper formulations with excellent thermal and oxidant stability. Importantly, these particles are uniquely suitable to prepare highly conductive Cu films at room temperature as opposed to conventional high temperature induced sintering, paving the way for more stable and practical Cu based flexible electronics.

## Mesh Bias Controlled Synthesis of TiO<sub>2</sub> and Al<sub>0.74</sub>Ti<sub>0.26</sub>O<sub>3</sub> Thin Films by Mist Chemical Vapor Deposition and Applications as Gate Dielectric Layers for Field-effect Transistors

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## Abstract

The effect of applying a mesh bias on the synthesis of amorphous titanium oxide (a-TiO<sub>2</sub>) thin films via mist chemical vapor deposition (mist-CVD) was investigated. When a negative bias is applied to the upstream electrode, some of the large mist particles are captured by the mesh electrode, promoting the generation of fine mist particles and increases the number density, resulting in a smooth and dense a-TiO<sub>2</sub> network. As a result, the rate of deposition of the a-TiO<sub>2</sub> thin films and the surface roughness decreased. The dielectric constant of the a-TiO<sub>2</sub> film also increased from 48 to 57.5. These findings suggest that in the synthesis of a-TiO<sub>2</sub> by mist-CVD is promising for promoting the densification of a-TiO<sub>2</sub> networks and for improving the junction properties at the a-TiO<sub>2</sub>/c-Si interface. The effect of applying a mesh bias on the synthesis of amorphous aluminum titanium oxide (a-Al<sub>0.74</sub>Ti<sub>0.26</sub>O<sub>3</sub>) thin alloy films is also a major subject of this study.

## Electrochemical Growth of Optical Active Noble Metal Nanolayers

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## Abstract

An ongoing goal in the field of optical nanotechnology is the creation of specific nanostructures by precisely engineering their physicochemical properties. Several scientific studies have already attempted to produce new structures from precious metals with new optical properties while maintaining electrical and thermal conductivity. In this context, the chemical and electrochemical synthesis and characterization of the sensor-active metallic nanostructures in aqueous and non-aqueous media will be presented. The porous noble metal nanostructures produced are of high purity and are characterized by broad absorptivity and low reflectivity in the ultraviolet, visible, and infrared range from 200 nm to 20,000 nm. X-ray analysis confirmed the purity and crystalline character. The electron micrographs show that the nanostructures consist of merged crystals forming porous assemblies. The properties of high conductivity, low reflection paired with a high specific surface make the porous noble metal nanosheets excellent candidates for applications in catalysis and optical sensors.

## Tunable Ferroelectric to Antiferroelectric Phase Transition by Intercalated Buffer Domain Walls in 2D Bismuth Tellurite

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## Abstract

Ferroelectric (FE) materials, showing switchable electrical polarizations under external electric fields, have shown great potential in applications of non-volatile memories, field-effect transistors, transducers, actuators, and other devices. In 2D materials, layers with distinct structural properties can be stacked and utilized for FE heterostructure

devices without limitation of substrate epitaxy, providing a wide range of tunability of the FE properties. However, the demand for further device miniaturization and fast access speed calls for smaller size of domains and easier control of polarizations in FE materials. Thus, domain and phase engineering become essential in 2D FE materials.

Here, we report the successful growth of few-layer 2D Bi<sub>2</sub>TeO<sub>5</sub> flakes by CVD method. Combining piezoelectric force microscopy, aberration-corrected scanning transmission electron microscopy and first-principles calculations, we unambiguously identified intrinsic in-plane ferroelectricity in few-layer Bi<sub>2</sub>TeO<sub>5</sub> flakes and discovered an intercalated buffer layer consist of mixed Bi/Te columns that serves as 180° domain wall, which can be facily intercalated into the FE matrix and lead to continuously variable polarized domain sizes. As the ultimate intercalated concentration where individual polarization domain approaches to half unit cell limit, a ferroelectric-antiferroelectric phase transition occurs. Moreover, the control of domain wall concentration can be realized by changing the ratio of the Bi<sub>2</sub>O<sub>3</sub>/Te precursors. The intercalated buffer domain wall provides a new paradigm in controlling the size and shape of the FE domains and FE-AFE transition in 2D FE materials, which tailors the functionalities in vdW materials and brings benefit for future utilizations in electronics.

## Physics of Atmospheric-pressure Acetylene Radiofrequency Micro-discharge: Effects of Dilution Gas and Gas Flow

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<sup>2</sup>*School of Science, Qiqihar University, People's Republic of China*

### Abstract

In this presentation, the effects of inert dilution gas and reactive gas flow on the dynamics of an atmospheric-pressure acetylene radiofrequency micro-discharge plasma will be reported. Due to the advantages of simplicity and low cost, this plasma source is widely used in the manufacturing of hydrogenated amorphous carbon (a-C:H) thin film. This film coating technology has attracted considerable interest in the fields of tribological materials, passivation layers, and field emission cold cathodes, due to their extraordinary material properties of high hardness, low abrasive coefficient, and chemical inertness. Due to the chemical complexity of acetylene gas, the fluid model is used to investigate its plasma property. Besides, due to the physical electron affinity, the nanoparticle is formed in the discharging process. Investigation of nanoparticle is also very important to the industry since it can be either beneficial or harmful to the production. So, the fluid model includes both the discharge plasma model and nanoparticle grow model. The plasma fluid model consists of the electron transport equation, ions equation, neutral equation, and the Poisson's equation. When further considering the gas flow effect, the background gas advection and heat process equations are included as well. The main discovery is the acetylene discharge is dominated by the famous electronegative bulk drift and ambi-polar field discharge mode and modulated by the dilution argon and helium; and the gas advection and heat process of background reactive gas, acetylene, is determined by the mutual transition between the gas internal and kinetic energies.

## A Study on the Temperature Sensitivity of Nanosensors Based on Single-walled Carbon Nanotubes in Ambient Conditions

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### Abstract

Electron transport in non-isolated carbon nanotubes is highly influenced by their interactions with their environment. In this study, the effect of the local surroundings on the temperature sensitivity of single-walled carbon nanotubes is investigated at ambient temperature. For this study, carbon nanotubes are trapped in between two nanoelectrodes

on a sapphire substrate using a dielectrophoretic trapping process. We find that it is possible to tune the temperature sensitivity by controlling the number of trapped nanotubes. The results indicate that the temperature sensitivity increases as the number of nanotubes decreases. For a device fabricated with a few carbon nanotubes resistance changes at a rate of 3.24%/°C but the sensitivity of devices with many carbon nanotubes is significantly smaller with a resistance change of 0.19%/°C. We attribute this effect to changes in the interaction of the sapphire substrate with changes in the carbon nanotubes' concentration.

## Magnetic Anisotropy Reversal Driven by Structural Symmetry-breaking in Monolayer $\alpha$ -RuCl<sub>3</sub>

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### Abstract

Layered  $\alpha$ -RuCl<sub>3</sub> is a promising material to potentially realize the long-sought Kitaev quantum spin liquid with fractionalized excitations. While evidence of this state has been reported under a modest in-plane magnetic field, such behaviour is largely inconsistent with theoretical expectations of spin liquid phases emerging only in out-of-plane fields. These predicted field-induced states have been largely out of reach due to the strong easy-plane anisotropy of bulk crystals, however. We use a combination of tunnelling spectroscopy, magneto-transport, electron diffraction and ab initio calculations to study the layer-dependent magnons, magnetic anisotropy, structure and exchange coupling in atomically thin samples. Due to picoscale distortions, the sign of the average off-diagonal exchange changes in monolayer  $\alpha$ -RuCl<sub>3</sub>, leading to a reversal of spin anisotropy to easy-axis anisotropy, while the Kitaev interaction is concomitantly enhanced. Our work opens the door to the possible exploration of Kitaev physics in the true two-dimensional limit.



## Young Researchers Presentations

### Oxide Thin Films for Next Generation DRAM Capacitor Electrodes via Atomic Layer Deposition

Se Eun Kim<sup>1,2\*</sup>, Ye Won Yun<sup>1,2</sup>, Hye Min Lee<sup>1,2</sup>, Byoung June Jun<sup>1,2</sup> and Sang Woon Lee<sup>1,2</sup>

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#### Abstract

Electrical devices such as laptops, tablets, and smartphones enable data processing, enriching our lives. As data throughput continues to increase, the demand for fast data processing has expanded. Therefore, when the CPU operates, a core memory that can transfer data at a high speed is required, and high density dynamic random-access memories (DRAMs) are currently playing this role.

DRAM stores data by distinguishing between the charge state of the capacitor. Since the size of DRAM cell is decreasing continuously for high density memories, its cell capacitance is decreasing. To increase the cell capacitance, high-k (high dielectric constant) thin films based on perovskite-structures such as SrTiO<sub>3</sub>, and (Ba,Sr)TiO<sub>3</sub> owing to their ionic polarizations in metal-insulator-metal capacitors. Currently, TiN is used for the metal thin films as electrodes. However, nitride-based electrodes are oxidized at the interface with high-k films, and a formation of dead layer at the interface between high-k/electrode causes a severe degradation in the achievement of high capacitance. Due to the high aspect ratio of DRAM capacitors, it is essential to deposit the high-k/electrode thin films using atomic layer deposition (ALD) with excellent step coverage.

Here, we present a deposition of oxide thin films by ALD for which minimize the degradation of interface at high-k/electrode thin films for next generation DRAM capacitors. For example, SrTiO<sub>3</sub> thin films were grown on perovskite-structured oxide electrode such as SrRuO<sub>3</sub> which showed a high capacitance. Besides the SrRuO<sub>3</sub>, we discuss another electrode using transition metal, vanadium dioxide (VO<sub>2</sub>).

### Enhanced Resistive Switching in Conductive Bridge Random Access Memory Using Two-dimensional Electron Gas at the Interface of Oxide Heterostructure

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#### Abstract

Resistive switching random access memory (ReRAM) has attracted considerable attention as the next generation non-volatile memory alternative to replace "FLASH" memory because of its fast-switching speed and high-density data capacity through the fabrication of its crossbar array architecture. A conductive bridge random access memory (CBRAM) is one example of ReRAM which has received significant interests. Unfortunately, previous CBRAM devices revealed a non-uniform resistance switching characteristics due to the uncontrolled formation and rupture of the filament under repetitive electrical stimuli. Here, we demonstrate highly uniform resistive switching devices using two-dimensional electron gas (2DEG) at the interface of an Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> thin film heterostructure via atomic layer deposition (ALD) as an electrode in CBRAM. The cell is composed of Cu/Ti/Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> where Cu/Ti and Al<sub>2</sub>O<sub>3</sub> overlayers are used as the active/buffer metals and solid electrolyte, respectively.

2DEG was observed at the epitaxial interface of oxide heterostructures such as LaAlO<sub>3</sub>/SrTiO<sub>3</sub>. The electrons are confined within 1~2 nm of out-of-plane direction near the Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> interface while they move freely along the in-plane direction. We show that 2DEG can be created in a non-epitaxial interface of the Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> heterostructure using ALD. High-density electrons up to 10<sup>13</sup> ~ 10<sup>14</sup>/cm<sup>2</sup> are confined at Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> interface which is similar to that of the epitaxial LAO/STO heterostructure. By using 2DEG, we demonstrate highly uniform resistive switching characteristics CBRAM. It exhibits a cycle endurance over 10<sup>7</sup> cycles.

Finally, we will introduce a hydrogen sensing application of the CBRAM devices for the first time which exhibited outstanding gas sensing performances.

## Epitaxial Growth of $V_2AlC$ Thin Films to Overcome Resistivity Increase for Next Generation Interconnects

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### Abstract

Copper (Cu) has been widely used as interconnect material in semiconductor devices. However, there are reliability problems such as electromigration and stressmigration because of high-density integration for high-performance of semiconductor devices. For the high-density integration, it is necessary to explore alternative metal materials to replace Cu because the resistivity of Cu film rapidly increases with decreasing physical size of interconnect in the semiconductor devices.

The problem of 'size effect' in resistivity is due to the increased grain boundary scattering and surface scattering in the small size of interconnects. In this respect, a low bulk resistivity ( $\rho_0$ ) with a short mean free path is advantageous in the size effect for interconnect applications (<10 nm). Recently, it has been reported that the characteristic parameter  $\rho_0 \cdot \lambda$  of  $V_2AlC$ , one of the  $M_{n+1}AX_n$  phases, is as low as  $4 \times 10^{-16} \Omega \cdot m^2$ , which is lower than that of Cu.

This research demonstrates a significantly reduced the size effect in resistivity using an epitaxial  $V_2AlC$  thin films grown by sputtering process on sapphire substrates. The *in-situ* crystallized  $V_2AlC$  thin films showed high-quality epitaxial properties.  $V_2AlC$  thin films showed a significantly weaker dependence on the film thickness than conventional metal films that resulted in a resistivity increase of only 20%, as the  $V_2AlC$  film thickness decreased from approximately 45 to 5 nm. This is owing to the highly ordered crystalline quality and small electron mean free path which has great potential in advanced metal technology to overcome the current scaling limitations of semiconductor devices.

## Design and Fabrication of Efficient n-MoS<sub>2</sub>/c-Si(p) Heterojunction Solar Cells

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### Abstract

For a practically functional solar cell, the cost-effectiveness and efficiency of the device is essential. Molybdenum disulfide (MoS<sub>2</sub>) has attracted great interest because of its significant chemical and physical properties. MoS<sub>2</sub> exhibit excellent charge carrier transport properties, i.e., high mobility values. Experimentally, carrier doping levels of  $10^{20} \text{ cm}^{-3}$  have been achieved in MoS<sub>2</sub> which makes it a potential low-cost and promising candidate for replacement of doped emitter layers in c-silicon (Si) solar cells. In addition, thin films of MoS<sub>2</sub> can be synthesized over a large area by the dual zone chemical vapor deposition (CVD) method without using any toxic gases. Motivated by the potential of the n-type MoS<sub>2</sub> (20 nm) /p-type crystalline-Si (275  $\mu\text{m}$ ) solar cell, thin films of MoS<sub>2</sub> were deposited on a p-type Si substrate using dual zone CVD technique. The resulting device (ITO/n-MoS<sub>2</sub>/c-Si (p)/Al/Ag) yielded an efficiency of 3.33 % with  $J_{sc}$  of 40.61 mA/cm<sup>2</sup>, FF = 0.30 and  $V_{oc}$  = 0.29 V. Simulation studies have been also performed to design magnesium fluoride (MgF<sub>2</sub> - 65 nm) /Indium tin oxide (ITO - 55 nm) based antireflection coatings for this device. The simulation studies suggested a significant improvement in the device efficiency is possible because of the reduced reflectance values. Further studies are going on for fabrication of Antireflection coating for improving the efficiency of device.

## A Novel, Greener Semiconductor – PEDOT: Carrageenan

## Zhongan Duan<sup>1,2\*</sup>, Simon Woodward<sup>1</sup>, Oleg Makarovskiy<sup>2</sup>, Michael P. Weir<sup>2</sup> and David B. Amabilino<sup>3</sup>

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### Abstract

There is an increasing opportunity for applying green and sustainable concepts in rapidly developing novel organic technologies with applications of organic electronic devices. The use of high conductivity and transparency conducting polymers to act as the charge transport layers or electrical interconnects in organic devices is widespread. PEDOT:PSS is a well-known, conducting polymer used in a range of diverse applications. Because of its high transparency, tuneable conductivity, and excellent thermal stability. However, PSS's resistance to acids, bases and photo-oxidation lead to environmental persistence. Thus, carrageenan (Carr), a more green and renewable material is considered to substitute PSS.

The aim of this work is to synthesis a conducting polymer, PEDOT:Carr, composed of PEDOT and two different types of Carr ( $\kappa$ - and  $\lambda$ -Carr) which act as counter ions. The synthesis is based on the simple chemical oxidation of the EDOT monomer in water. This polymer composite is then purified and subsequently drop-cast to fabricate films on various substrates. The concentration of the dispersion, degree of sulfation of the carrageenan dopant, the inorganic salt content of the dispersion and the ratio of Carr to EDOT were all investigated. The PEDOT:Carr suspensions and films were characterised using various techniques to understand the chemical and structural properties. The PEDOT:Carr films in this work exhibited good conductivity and thermal properties. Therefore, the synthesised composite was used in combination with various n-type materials in the fabrication of thermoelectric devices. The results are promising which show this PEDOT:Carr composite to be an attractive, sustainable alternative conducting material for a range of functionalities.

## Synthesis and Characterisation of Asymmetric Perylene-based Supramolecular Polymers

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### Abstract

Supramolecular polymers (SMPs) are a unique class of materials, which are held together by non-covalent and highly directional interactions. SMPs and conventional polymers possess common properties, such as low viscosity. However, owing to the reversibility of non-covalent interactions, SMPs exhibit significantly more dynamic behavior, enabling them to display various properties such as self-healing, processability, and stimuli-responsiveness. Perylene diimides (PDIs) have attracted attention as building blocks for SMPs through solution self-assembly. PDIs feature a range of attractive properties, including optoelectronic properties, that enables the investigation of their self-assembly, thermal, and photochemical stability, easy chemical modification, and widespread potential applications. Modification on the imide position is one of the strategies for designing novel functional PDIs. Asymmetric PDIs with different substituents at each imide position are an essential subgroup within this class of compounds owing to their substantial synthetic versatility, and have not been explored in great details for their self-assembly behavior. In this work, we aim to explore the formation of SMPs based on asymmetric PDIs by targeting the imide positions on perylene tetracarboxylic dianhydrides. Different asymmetric PDIs have been successfully synthesised using a variety of hydrophilic/hydrophobic amines. We expect to design novel SMPs based on asymmetric PDIs and explore their self-assembly mode, behaviour and resulting supramolecular structures.

## Atomic Layer Deposition of Nickel Thin Film for Low Resistivity Metal Application

## Sang Mo Moon\*, Hye Min Lee, Ju Young Sung, Chae Hyun Lee and Sang Woon Lee

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### Abstract

Metal plays an important role in semiconductor devices for electrodes and interconnects. Recently, as integration density of semiconductor devices becomes higher, the scaling-down of metal components is inevitable, causing substantial resistivity to increase by electron scattering in the metal thin films which is known as the “size effect” of resistivity. The size effect of resistivity in metal thin films is a serious problem in integrated circuits because it causes RC delays and performance degradation. Metal thin films with a lower bulk resistivity ( $\rho_0$ ) and a shorter mean free path (MFP) is advantageous in maintaining low resistivity in small scales (<10 nm). Ni thin films showed low resistivity at the thin-thickness range (<10 nm) which was significantly lower than that of conventional metal thin films (Cu, Al, etc.). This is due to the short MFP (~6 nm) and low bulk resistivity (6.9  $\mu\Omega\cdot\text{cm}$ ) of Ni.

In this study, a high-purity Ni thin film was deposited by atomic layer deposition (ALD) process for electrode and interconnect applications. Nickel(II) 1-dimethylamino-2-methyl-2-butoxide, Ni(dmamb)<sub>2</sub> with NH<sub>3</sub> as reactant was employed in ALD of Ni thin films. Ni<sub>3</sub>C and pure Ni phases were identified depending on ALD conditions, and low resistivity Ni thin films were obtained by ALD process optimization. In the presentation, the material properties of ALD Ni thin films including crystallinity, impurity contents, and electrical properties are discussed, showing potential merits of films for electrode and interconnects to overcome material scaling limitations.

## Growth of Epitaxial NbN Thin Films Using Atomic Layer Deposition on Cubic MgO Substrate

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### Abstract

Dynamic random-access memories (DRAMs) play crucial roles in present computing systems with logic devices. In DRAMs, data 0 and 1 are expressed according to the potential level of the electric charge stored in the capacitors. Recently, the leakage current through high-k (high dielectric constant) thin film in metal-insulator-metal type DRAM capacitors keeps increasing which leads to a failure in the memory operation. Therefore, it is necessary to reduce leakage currents using metal thin films with a higher work function than that of conventional TiN thin films.

Here, we present an alternative metal thin film NbN for advanced DRAM capacitors. The NbN thin films could be grown epitaxially by atomic layer deposition (ALD) using NbCl<sub>5</sub> (Nb precursor) and NH<sub>3</sub> (nitrogen source) at a deposition temperature of 450 °C. The cubic NbN thin film was grown coherently on a cubic MgO substrate owing to a small lattice matching between NbN and MgO. A polycrystalline-NbN thin film grown on the SiO<sub>2</sub> substrate showed a high concentration of Cl impurities (4 - 5%). However, the concentration of Cl impurities in the epitaxial grown NbN thin film decreased to ~2%, which promoted the epitaxial growth of the NbN film on the MgO substrate. Since a tensile strain was observed at the NbN/MgO interface, it was anticipated that Cl desorption was promoted during NbN ALD. With the epitaxial growth of NbN thin films, it allowed 50% lower resistivity of NbN thin films than polycrystalline NbN thin films due to increased carrier mobility via reduced carrier scattering.

## Alternative Surface Reaction Pathways in Atomic Layer Deposited NbN Thin Films for Reduced Resistivity

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### Abstract



Transition metal nitride thin films, such as titanium nitride (TiN), are essential for electrode thin films in memory and transistor devices. NbN thin films have attracted attention for replacing TiN thin films as capacitor electrodes in advanced dynamic random-access memories (DRAMs) owing to their higher work function ( $> 4.7$  eV) than that of TiN ( $\sim 4.5$  eV) which allows a reduced leakage current in DRAM capacitors. Due to the high aspect ratio of DRAM capacitors, it is essential to deposit the electrode thin films using atomic layer deposition (ALD) with excellent step coverage.

To manufacture advanced DRAM capacitors, the process temperature of the bottom electrode thin films must be lowered to  $400$  °C due to process temperature limitations. However, the conventional NbN ALD process using  $\text{NbCl}_5$  (Nb precursor) and  $\text{NH}_3$  (nitrogen source) results in high resistivity ( $> 500$   $\mu\Omega\cdot\text{cm}$ ) due to the residual impurity concentration ( $> 5\%$ ) at a process temperature of  $400$  °C. To solve this issue, we propose an alternative ALD surface reaction pathway by introducing  $\text{H}_2\text{S}$  gas pulses between the  $\text{NbCl}_5$  and  $\text{NH}_3$  pulse steps to reduce the Cl impurity concentration. Our findings demonstrate that this alternative ALD reaction successfully reduced the residual Cl concentration to below  $1.5\%$  (decrease by  $> 50\%$  at the identical ALD process temperature). The reduced Cl impurity enabled a decrease of resistivity (greater than  $30\%$ ) of NbN thin films at  $400$  °C compared to conventional NbN ALD.

## Functional Materials Based on Lanthanide(III) Monoporphyrinates Complexes with Potential Applications in Optoelectronic and Nanoscale Rotors

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<sup>2</sup>Laboratory of Liquid Crystals, Department of Organic Chemistry, Faculty of Chemical Sciences, University of Concepción, Chile

### Abstract

Molecular architectures play a fundamental role in the quest to miniaturize electronic and mechanical devices [1]. In general, systems based on coordination compounds represent an attractive target for the development of molecular functional materials manipulable at the nanoscale due to their structural versatility, improved electronic properties due to the presence of the metal center, added to their high chemical and thermal stability [2]. The use of lanthanides(III) monoporphyrinates containing dipolar ancillary ligands, allows the access and study of novel coordination complexes with potential applications as technomimetic molecular design with respect to a propeller-type rotor. The porphyrin fragment is immobilized on a metal surface, e.g., Au(111), and it is possible to induce rotation of the auxiliary ligand around the metal center using Scanning Tunneling Microscopy [3]. In this regard, the dipolar moment due to the presence of electro-donor (D) and electro-acceptors (A) terminal groups linked by a p-conjugated bridge (D-p-A) in the rotator ligand, orientates the molecules in the solid state allowing the synchronized manipulation of molecular arrays deposited on a surface [4]. In addition, the electronic nature of these molecular fragments (D-p-A), will give access to chromophores with second-order nonlinear optical activity (ONL-2) in solution and the solid state by second harmonic generation [5]. Considering these points, we present the synthesis and study of these molecular entities allows access to multifunctional molecular materials, with potential applications in optoelectronics and mechanical devices at the nanoscale. All molecular entities were studied and characterized by: UV-Vis, FT-IR, <sup>1</sup>H- and <sup>13</sup>C-NMR, ESI-MS, and single-crystal XRD.

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## Self-powered Thermistor Based on Semiconducting Ferroelectric SbSI Nanowire

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### Abstract

Since ferroelectric materials are semiconductors themselves and promising materials for energy harvesting, nanogenerators based on the semiconducting ferroelectric materials are profitable self-powered systems with high performance. Integrating NTC thermistors consisting of semiconducting ferroelectric material with nanogenerators that harvest energy provides improved convenience and battery-free temperature sensing, which can be utilized in diverse home or industrial applications for monitoring temperature variations immediately. This work processed AV-BVI-CVII semiconductor group SbSI nanowire using a typical sonochemical synthesis. The structural, morphology, and electrical properties of SbSI based pellet were investigated to confirm the phase formation and dielectric parameters. The thermal coefficient of resistance varied from -0.16%/K to -0.31%/K. The thermal sensitivity of SbSI based thermistor was evaluated corresponding to the working temperature changing from 20 °C to 80 °C. The characteristics of the thermistor for measuring temperature can offer better resolution and high accuracy in a specific range of temperatures. We developed SbSI nanowire/Kapton TENG to monitor the temperature change. The SbSI thermistor warns if the temperature is beyond the human adjustable range with the output signals. This work paves the way for designing new lead-free materials for energy harvesting and self-powered applications.

## On the Way to Improve Eco-friendly Silver Bismuth Iodide Photovoltaic Cells. Challenges and Prospectives

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### Abstract

Perovskite-inspired Silver Bismuth Iodide (ABI) with the structure  $A_a B_b I_{x=a+3b}$  (A = Ag; B = Bi) exhibits a desirable bandgap between 1.8 - 1.9 eV, strong absorption characteristics, and environmental friendliness attributed to the lower toxicity of bismuth being a promising alternative to Pb-perovskites [1].

Several compounds with different compositions such as  $Ag_3BiI_6$ ,  $Ag_2BiI_5$ ,  $AgBi_2I_7$  have been used for photovoltaic applications, however, despite extensive research efforts, these materials exhibit on average a very low current density ( $J_{sc}$ ) and open-circuit voltage ( $V_{oc}$ ) producing performance range between 2 - 4% while their theoretical limit, estimated based on the bandgap of 1.86 eV for  $Ag_2BiI_5$  is 25%. This evinces a major intrinsic loss of carriers in the material which needs to be identified in order to understand and improve ABI performance.

In this presentation, we introduce our advances with ABI. First, we will talk about their use in as absorbers in solar cells. Then, a deep understanding of different  $AgI:BiI_3$  ratios for improvement of PCE of n-i-p cells with the structure ITO/SnO<sub>x</sub>/ABI/PTAA/Au will be discussed. Using an optimal  $AgI:BiI_3$  ratio of 2:1.5 we achieved a

power conversion efficiency (PCE) of 2.1% with a  $V_{oc}$  of 0.8 V, one of the highest reported so far for this material [2]. Also, we will show their potential for indoor applications, and report 5% PCE for semi-transparent ABI-based solar cells. In the end, we will present some advances related to basic research for the intrinsic losses of ABI. Through UV-Vis measures on ABI solutions, we were able to detect the presence  $[BiI_{3+x}]^{-x}$  complexes that potentially could influence the crystallization leading to impurities.

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## Effect of Rare Earth (RE<sup>3+</sup>) Ionic Radii on Transparent Lanthanide-tellurite Glass-ceramics: Correlation Between ‘Hole-formalism’ and Crystallization

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## Abstract

Rare earth (RE) doped transparent tellurite glass-ceramics (GCs) are the most promising material for advanced photonic applications. Specifically, the growth of RE based “anti-glass” crystallites in transparent GCs enhances their effective functionality. Optimization of glass composition and heat-treatment schedule are the foremost factors that affect the transparency of GCs. Nevertheless, the direct effect of RE<sup>3+</sup> ions on the crystallization mechanism of glass has hardly been reported. Therefore, a base glass of La<sub>2</sub>O<sub>3</sub>-Gd<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub>-TeO<sub>2</sub> (LGTT) is doped with RE<sup>3+</sup> ions (Ce<sup>3+</sup>, Pr<sup>3+</sup>, Nd<sup>3+</sup>, Sm<sup>3+</sup>, Eu<sup>3+</sup>, Tb<sup>3+</sup>, and Dy<sup>3+</sup>) having varied ionic radii. Rietveld refinement of GCs confirmed that (La/Gd)<sub>2</sub>Te<sub>6</sub>O<sub>15</sub> phases are precipitated, where dopant Ce, Pr and Nd occupy La sites, while Sm, Eu, Tb, Dy occupy Gd sites. The configurational heat-capacity ( $\Delta C_p$ ) from DSC is found to be lower for larger ionic radii REs (Ce, Pr, and Nd) than smaller ionic radii REs (Sm, Eu, Tb, and Dy) thereby exhibiting higher chemical ordering followed by faster crystal growth rate in glass. However, transparency retention profile of different RE-doped GCs are following the trend, Eu:Tb>Sm:Dy>Nd>Pr>Ce, which confirms that ionic radii alone are not the influencing factor. In this study, we proposed ‘Hole-Formalism’ concept along with ionic radii effect to explain the observed trend. According to ‘Hole-Formalism’ concept it is expected that RE ‘Hole-Pairs’ ( $4f^n \equiv 4f^{14-n}$ ) would show similar structural occupancy as well as identical crystallization tendency. It is further corroborated with  $\Delta C_p$  values for Sm<sup>3+</sup>:Dy<sup>3+</sup> ( $4f^5:4f^9$ ) and Eu<sup>3+</sup>:Tb<sup>3+</sup> ( $4f^6:4f^8$ ) ion pairs, resulting similar crystallization mechanism, transmission profile and fine-scale microstructures of these RE-based GCs.

## Spin Teorientation to a $\Gamma_3(C_x, F_y, A_z)$ Configuration and Anisotropic Spin-phonon Cou-

## pling in a $\text{Sm}_{0.5}\text{Y}_{0.5}\text{FeO}_3$ Single Crystal

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### Abstract

This study reveals an unusual temperature induced spin reorientation transition in single crystal  $\text{Sm}_{0.5}\text{Y}_{0.5}\text{FeO}_3$ , rare earth orthoferrite. The transition is observed from  $\Gamma_2$  to  $\Gamma_3$  spin configuration near room temperature, in the temperature interval of 282 - 312 K. After the transition, the weak ferromagnetic moment of  $\text{Fe}^{3+}$  remains along a-axis till Neel temperature ( $T_N = 654$  K). The findings of our investigations reveal the potential of  $\text{Sm}_{0.5}\text{Y}_{0.5}\text{FeO}_3$  system to be a vital material in spintronic devices due to room temperature spin reorientation transition. The striking changes associated with the Raman modes in temperature dependent Raman studies, confirm the directional change in the reorientation of spin lattice structure. Additionally, magnon-spectral peaks observed in polarized Raman investigations reaffirm the reorientation of spin configuration and the anisotropy associated with the transition. Temperature-dependent Raman data reveal the involvement of strong spin-phonon coupling facilitated by exchange striction in driving the unusual spin reorientation transition in  $\text{Sm}_{0.5}\text{Y}_{0.5}\text{FeO}_3$  single crystal.

## Coherent Phonon Dynamics in Non-centrosymmetric Potassium Titanyl Phosphate Crystal

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### Abstract

Potassium titanyl phosphate (KTP) is widely used as a nonlinear gain material in harmonic and broadly tunable lasers and is used for various electro-optic applications, including active waveguides, due to its higher nonlinear coefficients and high damage threshold. In this study we present results on direct time-dependence of the phonon decay in a non-centrosymmetric KTP crystal using Coherent Anti-Stokes Raman Scattering (CARS) technique where three-color tunable femtosecond pulses provided the phonon decay transient detection up to a signal to noise ratio of 70 dB. The equivalent spectral resolution was better than  $0.15 \text{ cm}^{-1}$  and the decay of the Raman active vibrations has been traced in time with  $<120$  fs resolution. Ultrafast time resolution and superb sensitivity of CARS technique provided valuable insight into the dynamics of Raman active vibrations within the frequency range of  $260 - 1070 \text{ cm}^{-1}$ , that belong to octahedral titanium ( $\text{TiO}_6^-$  oxide group) and tetrahedral phosphate ( $\text{PO}_4^-$  oxide groups) sites. The observed phonon decay rates were in range  $0.93 - 4.25 \text{ ps}^{-1}$  with respective linewidths of  $4.9 - 22.3 \text{ cm}^{-1}$ . The damping rate is a key parameter that influences the efficiencies of the second- and third-order nonlinear processes in laser frequency conversion devices. The obtained information is valuable from the perspective of problems in fundamental condensed matter physics such as parametric interactions within crystal lattice due to nonlinear potential. This material is based upon the work supported by the United States Air Force Office of Scientific Research under Award No. FA9550-18-1-0273.

## Poster Presentations

### Effect of RF Magnetron Growth Conditions on Bismuth Ferrite Based Thin Film

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#### Abstract

The multiferroic, catalytic and optical properties of bismuth ferrite encouraged their study and applicability in spintronics, data storage devices, pollutant removal, etc. The structural, magnetic and electric characteristics of bismuth ferrite-based materials vary significantly, primarily on the shape of the samples and furthermore on the synthesis conditions. In our study, bismuth ferrite based thin films were grown on silicon and quartz substrates by RF magnetron sputtering in different conditions of substrate temperature (room temperature – 700 °C), mixt gas pressure (0.5 Pa - 3 Pa) and Ar:O<sub>2</sub> ratio of the background gas (3:1 - 50:1 and without O<sub>2</sub>). The structural analysis results revealed that for substrate temperatures below 500 °C the depositions were amorphous and at 700 °C residual phases were detected. The diffraction lines of the film deposited at 600 °C were associated with Bi<sub>2</sub>Fe<sub>4</sub>O<sub>9</sub> and Bi<sub>25</sub>FeO<sub>40</sub> phases. The increase in mixt gas pressure showed an improved crystallinity of the samples up to 1 Pa while at higher pressured the films were amorphous. The use of low O<sub>2</sub> background gas during the deposition determined a phase transformation process. Chemical composition measurement revealed a uniform distribution of the main elements and showed stoichiometry changes with pressure variations. The optical band gap values obtained by Tauc plot from UV-Vis spectroscopy measurements were not influenced by the substrate temperature but by the pressure of the Ar:O<sub>2</sub> gas. The magnetic properties were correlated with the structural characteristics and the highest magnetic response was observed for the film deposited at 600 °C, 1 Pa and 3:1 Ar:O<sub>2</sub> gas pressure.

### ZnO Nanoparticles Loaded with Essential Oils as Antimicrobial Agent for Food Packaging

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#### Abstract

ZnO nanoparticles (NPs) present antimicrobial activity, while being considered safe. At the same time the plant extracts are gaining ground as potential – future antimicrobials, with broad spectrum of activity and without drawbacks of antibiotics. By combining two antimicrobial agents, a synergic activity can be obtained, allowing either decrease of the antimicrobials amount or a stronger activity. In this paper we report the ZnO NPs loading with ten different essential oils (EO) and the antibacterial activity against some usual food-borne pathogens *Listeria monocytogenes*, *Staphylococcus aureus*, *Salmonella typhimurium*, and *Escherichia coli*. Such nanosystems can be incorporated further in food packaging allowing the increase of shelf life and food security. The EO used were: orange, thyme, lavender, grapefruit, citronellol, bergamot, cinnamon, limette, menthe, and rosemary. Strong antibacterial effect was observed for all the tested samples, confirming the synergic activity of ZnO NPs and EO.

## Acknowledgements

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## 2D Materials Modified with Metal-containing Ionic Liquid

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### Abstract

2D materials such as graphene-based or layered double hydroxides/alkoxides are often used as inorganic fillers for the improvement of the mechanical, and electrical properties of final polymeric composites. Layered double hydroxides could be also applied as catalysts depending on the composition. The ionic liquids could have also more functions for application in polymer chemistry. It could be used as a solvent, surfactant, catalyst, etc.

The metal-containing ionic liquids could be also applied as homogenous catalysts. It was important to study the influence of metals in imidazolium-based ionic liquids as well as the influence of aliphatic chains. The presented results will show the synthesis of imidazolium-based ionic liquids with different length of aliphatic chains and their thermodynamic study for application as homogenous catalysts. The ionic liquids will be also studied to modify 2D materials as graphene-based and some layered double hydroxides/alkoxides.

### Acknowledgements

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## Solid-state Alkoxides - Synthesis, Properties, and Applications

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### Abstract

Solid-state alkoxides contain simultaneously organic and inorganic components which give them unique properties. Commonly, these compounds contain elements from d-, f-, p-block of the periodic table. On the other hand, alkaline and alkaline earth alkoxides have not been reported often. Several synthetic methods as coprecipitation or solvothermal reactions have been employed to prepare solid-state alkoxides. Depending on the methods, various alcoholic groups could be introduced into the alkoxide to form for example ethoxide or glycerolate. The products were investigated for various applications, for example as catalysts or for further preparation of metal oxides with unique properties. Here we present several alkoxides prepared by the solvothermal method. Catalytic tests are also planned. Another set of experiments is designed to prepare compounds by removal of the organic component.

### Acknowledgements

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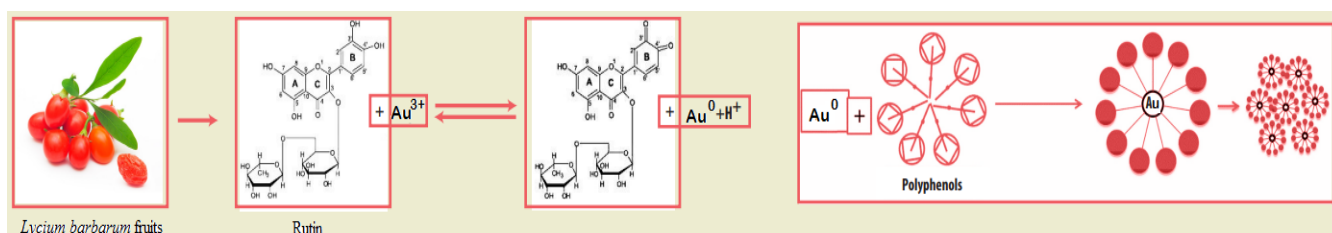
## Green Synthesis of New Biomaterials Based on Gold Nanoparticles and Phytocompounds from *Lycium barbarum* L. Fruits with Potential Antidiabetic Activity

B. Moldovan<sup>1</sup>, V. Morosan<sup>1</sup>, I. Baldea<sup>2</sup> and L. David<sup>1</sup>



<sup>1</sup>Babeş-Bolyai University, Faculty of Chemistry and Chemical Engineering, Romania<sup>2</sup>Faculty of Medicine, "Iuliu Hatieganu" University of Medicine and Pharmacy, Romania**Abstract**

The first phytomediated green synthesis of gold nanoparticles using fruits extracts was reported two decades ago. Phenolic compounds from fruits can act both as reducing and capping agents for metal nanoparticles. Several studies revealed the presence of high amounts of antioxidant polyphenolic compounds, such as rutin, in *Lycium barbarum* fruits (Figure). The extracellular synthesis of a novel hybrid biomaterial based on stable gold nanoparticles using polyphenols from goji (*L. barbarum* L.) fruit extract has been achieved (Figure). UV-Vis spectroscopy, transmission electron microscopy, and Fourier transform infrared spectroscopy were used to characterize the obtained nanoparticles. The *in vitro* protective effect of AuNPs against hyperglycemia-induced oxidative stress on endothelial cells was evaluated, in order to establish their potential applications in the therapy of diabetes.



**Figure:** *Lycium barbarum* mediated synthesis and stabilization of AuNPs.

## Catalytic Activity Against Harmful Azoic Dyes of Green Synthesized Silver Nanoparticles Using the Antioxidant Goji Berry Extract

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**Abstract**

Silver nanoparticles (AgNPs) were obtained in one step, green, nontoxic, rapid and economic method, using *Lycium barbarum* fruit extract as a source of reducing and stabilizing agents. UV-Vis spectroscopy, transmission electron microscopy, and Fourier-transform infrared spectroscopy, were used to characterize the newly obtained nanoparticles. The catalytic activity of the obtained nanoparticles was evaluated in the reductive degradation process of two azoic dyes used in the food industry: azorubine and tartrazine. The AgNPs mediated degradation of the dyes was proceeded 3.2 and respectively 1.6 times faster than in the absence of any catalyst (Figure).



**Figure:** Catalytic activity.

## Effect of ZnO Thickness on Gas Sensing Behavior of $\text{WS}_2$ -ZnO p-n Heterojunction Nanosheets Towards Reducing Gases

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## Abstract

Optimization of materials in heterojunction gas sensors is vital for achieving the highest gas-sensing performance. In this study, we synthesized pristine ZnO, pristine WS<sub>2</sub> nanosheets (NSs), and ZnO with different thicknesses (10 - 50 nm) on WS<sub>2</sub> NSs to study their gas-sensing properties. It was found that at 150°C and 300°C, the sensors with ZnO layers of 10 and 30 nm, respectively, exhibited the highest response to reducing gases. At low temperatures, the role of WS<sub>2</sub> in gas sensing was dominant, whereas at high temperatures, ZnO played a dominant role. Therefore, the sensor with the thinnest ZnO layer demonstrated the best performance at low temperatures, while at higher temperatures, the sensor with a ZnO thickness of 30 nm exhibited optimal performance. Also, at 300°C, WS<sub>2</sub> was oxidized to WO<sub>3</sub>. Furthermore, to decrease overall power consumption, we conducted sensing measurements under self-heating conditions on a WS<sub>2</sub>-ZnO (10 nm) p-n heterojunction NS sensor and found that the WS<sub>2</sub>-ZnO (10 nm) p-n heterojunction NS gas sensor, under a low applied voltage of 4.2 V, exhibited the highest response to reducing gases. The enhanced gas sensing of the optimized gas sensors was attributed to the formation of heterojunctions and the optimal thickness of the ZnO layer on WS<sub>2</sub> at appropriate temperatures.

## Synthesis of Chitosan-based Graphene Filter for Bioaerosols and Volatile Organic Compounds Removal

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### Abstract

Indoor air quality recently becomes an important issue of public health in the post-coronavirus disease (COVID-19) pandemic period. People are researching novel materials for air purification by removing bioaerosols and toxic volatile organic pollutants (VOC). Graphene (Gr) nanoparticles present antibacterial ability via oxidative and membrane stress on bacterial cell walls. Chitosan (CS) binds to the negatively charged bacterial cell wall and disrupts cells, thus altering the membrane permeability. The objective of this study is to develop a novel filter of air purifiers, equipped with CS-based Gr nanoparticles. The novel filter removes bioaerosols and VOC at the same time. As results, the novel CS-based Gr filter is successfully produced. The composition of CS, 3 nm or 12 nm Gr nanoparticles has been identified on the surface in filters. The antibacterial ability of filters on *Staphylococcus aureus* ranked as CS based-3 nm Gr (95.26%) > CS based-12 nm Gr (86.50%) > CS only (15.32%). A similar trend for removing high-density bioaerosols ( $5.35 \times 10^6$  CFU/m<sup>3</sup>) in the air purification, ranked as CS-3 nm Gr (98.06%) > CS-12 nm Gr (95.62%) > CS only (43.26%). The destroyed bacterial residues are observed on the SEM profile of CS-based Gr filters. Moreover, the saturated concentration of formaldehyde is removed by CS based-Gr filters. The removal rate of VOC was compared as follows: CS based 12 nm Gr ( $5.19 \text{ mg/m}^3 \times \text{min}$ ) > CS-based 3 nm Gr ( $5.14 \text{ mg/m}^3 \times \text{min}$ ) > CS only ( $3.60 \text{ mg/m}^3 \times \text{min}$ ). In conclusion, the CS based-3 nm Gr filter is suggested to use in air purifiers in the future, presenting the best antibacterial ability of bioaerosols.

## Surface Modified Ceria Nanoparticles with Amine-based Accelerator and its Influence on Chemical-mechanical Polishing Process

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### Abstract

Among the various factors influencing the polishing efficiency of Si-type chemical mechanical polishing (CMP), the extent of hydrolysis reactions occurring at the wafer surface due to water in the slurry leads to faster removal rates. Additives such as NaOH and KOH are commonly used in slurries to promote hydrolysis, and amine-based additives have been reported to enhance polishing efficiency more effectively. However, these polishing additives are typically dispersed in the slurry, which may result in wasteful utilization if they operate beyond the range where the

abrasive interacts with the wafer. Therefore, positioning the additive between the abrasive and the wafer optimizes its functionality. Moreover, strong covalent bonding between Si wafers and amine-based polishing additives can remove the polished wafer surface in the form of SiO<sub>2</sub> clusters, acting as chemical teeth to increase the removal rate at a macroscopic level. To address these limitations, in this study, we fabricated surface-modified ceria nanoparticles (pico-ceria) using picolinic acid, an amine-based polishing accelerator, to create CMP abrasive particles that selectively induce wafer planarization within the controlled range of physical interactions. The performance of the fabricated abrasive particles was evaluated. Pico-ceria was characterized using scanning electron microscopy, thermal gravimetric analysis, and spectroscopic techniques (<sup>1</sup>H NMR and FTIR). Slurries containing pico-ceria were adjusted to pH 4 and stabilized with the addition of PVA (Mw~1700) for dispersion stability. The polishing efficiency was measured on SiO<sub>2</sub> and Si<sub>3</sub>N<sub>4</sub> wafers.

## ZnFe<sub>2</sub>O<sub>4</sub> Nanoparticles for Gas-sensing Applications: Monitoring of Structural Parameters while Exposing the Ferrite in Gas Atmospheres

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### Abstract

This work presents a hydrothermal-based facile method for synthesizing ZnFe<sub>2</sub>O<sub>4</sub>, whose size can be controlled with the concentration of sodium acetate used as a fuel. The characterization of the morphology, structure, composition, and electronic properties of the synthesized samples is also presented. The crystal structure of the synthesized samples was determined using an X-ray diffractometer while scanning electron microscopy was used for the determination of the morphology of synthesized materials. It revealed that the particles possessed spherical morphology whose size decreased with the increasing sodium acetate amount. Transmission electron microscopy (TEM) was utilized to determine the structure, morphology, and elemental distributions in particles at the nanoscale. X-ray photoelectron spectroscopy and core-loss electron energy loss spectroscopy showed an increasing fraction of Fe<sup>2+</sup> with the decreasing size of the particles in samples. Brunauer-Emmett-Teller analysis of samples revealed a higher surface area as the particle size decreases. The *ab initio* calculations of the density of states and band structure of (001) surface terminating ZnFe<sub>2</sub>O<sub>4</sub> particles were carried out using Quantum Espresso software. They were compared to the experimentally determined bandgap values for the corresponding samples. Finally, *in-situ* TEM measurement was carried out on one sample and revealed that the lattice parameter of ZnFe<sub>2</sub>O<sub>4</sub> nanoparticles showed a noticeable fluctuation upon exposure to CO<sub>2</sub> and Ar gases. It is concluded that the size reduction of the nanoparticles tunes the bandgap and provides more active sites due to a higher concentration of oxygen vacancies.

## Detecting Low Dose of Glucose in the Microwave Range by Using Thermoelastic Optical Indicator Microscope

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### Abstract

In this study, we employed a non-invasive approach using a thermoelastic optical indicator microscope to investigate aqueous solutions of glucose. To enhance the interaction between electromagnetic waves and the material, we conducted measurements using a silicone rectangular container with dimensions matching the microwave beam diameter. The container was filled with varying concentrations of glucose within the range of 0 - 200 mg/dl. Throughout the testing process, we recorded and processed the maximum intensity and frequency response. These

results provide valuable insights for determining and monitoring glucose concentrations in aqueous solutions. Additionally, the findings present new opportunities for the development and production of highly sensitive non-invasive biosensors.

## Enhancement of Biological Properties of Endodontic Filling Material by Organic-inorganic Hybrid Material

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### Abstract

Organic-inorganic hybrid materials are a class of materials that combine organic and inorganic components at the certain level, resulting in enhanced or tailored properties. Mineral trioxide aggregates (MTA) have been shown to be highly useful as a biocompatible and bioactive material in conservative dentistry; however, it also has some critical drawbacks such as low mechanical properties, difficulty in handling, long setting time. hPDLF cells (Lonza, Basel, Switzerland) and hFOB (ATCC; Rockville, MD, USA) were used for this study. MTA (ProRoot MTA, Dentsply sirona, USA) was mixed with bioactive glass (63S BAG, Bonding Chemical, USA) as inorganic components and 10 wt.% elastin-like polypeptide (ELP) solution as organic material. To investigate the cell proliferation, MTT assay was conducted; for the mineralization effect of new experimental filling material, alizarin red S staining was performed; for the cell migration, wound healing assay and trans-well assay were performed. MTA 98 - 97%; BAG 2 - 3% with ELP sol) exhibited the prominent calcium deposit in ARS test and showed higher cell viability in MTT assay. The groups showed the faster growth into the wound and presented the higher migration rate in trans-well assay. MTA with incorporation of 2 - 3% BAG and ELP solution as inorganic-organic hybrid enhancement exhibited the superior bioactive performance in aspect of cell viability, hard tissue formation and soft tissue healing capabilities compared to original MTA.

## Preparation of Anticancer Metal Organic Frameworks Composed of Copper, Cobalt, and Zinc: Their Biocompatibility and Apoptosis Mechanism

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### Abstract

A metal organic framework (MOF) has a network structure consisting of metal clusters connected by organic linkers with high porosity and provides a desirable combination of structural features that can be adjusted with large cargo payloads along with Cu, Co, and Zn-MOF, which have the chemical stability required for water-soluble use. Bioactive MOFs containing Cu, Co, and Zn were prepared by modifying previous methods as a therapeutic drug. Their structures were characterized via PXRD, single crystal crystallographic analysis, and FTIR. The degradability of MOFs was measured in media such as deionized water or DPBS by PXRD, SEM, and ICP-MS. Furthermore, we investigated the anticancer activity against cell lines SKOV3, U87MG, and LN229 as well as biocompatibility toward normal fibroblast cells. The result shows that nanoporous 3D Cu-MOF could be a potential promising candidate for chemoprevention and chemotherapy.

## Modulating Corneal Endothelial Cell Response with Corneal Mimicking Substrates

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## Abstract

Currently, around 10 million people worldwide suffer from visual impairment caused by corneal diseases. The standard treatment involves corneal transplantation from donors, mainly due to failures in the corneal endothelium, an inner layer unable to regenerate naturally. However, this approach faces limitations like donor scarcity and immune rejection. Researchers is focused on the cultivation of corneal endothelial cells (CEC) as an alternative solution.

To address challenges linked with cell therapy viability after injection, tissue engineering has emerged as a promising field. It combines cells, biomaterials, and biological molecules to create functional tissues. Interestingly, different cell behaviors and functionalities can result from varying cell culture topographies, making this a crucial aspect in the field. This project employs tissue engineering to generate functional CEC, mirroring their natural characteristics. The strategy involves cultivating cells on substrates with diverse curvatures and topographies resembling those of the human eye.

A groundbreaking aspect of this work is the integration of native corneal tissue-mimicking materials to form curved substrates with specific topographies, utilizing a conventional 3D printer. The hypothesis revolves around the potential of such substrates to alter cell phenotype and behavior beneficially. Results highlight that curved patterned substrates rapidly enhance cell function and morphology, as indicated by markers ZO-1 and ATP1A1 expression.

In summary, this project introduces an innovative approach to enhance CEC culture by uniquely combining curved surfaces and microtopographies, mimicking the native environment.

## Improved Biophysical Properties and Controllable Gelation in Silk Fibroin/Collagen Hydrogels for Cell Encapsulation

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## Abstract

Tunable mechanical and biological qualities make cell-encapsulating hydrogels important for cell transport and tissue engineering. Cell culture hydrogels might be silk fibroin and collagen, two key biological proteins. Individually, however, the two have been employed despite their poor mechanical characteristics and cell-mediated shrinking (collagen) and absence of cell adhesion motifs (silk fibroin from *Bombyx mori* (mulberry)). Thus, combining them improves mechanical and biological qualities over separate hydrogels. We demonstrate that cell-encapsulating hydrogels of mulberry silk fibroin/collagen may be made in a variety of compositions by combining gelation methods. The silk fibroin/collagen hybrid hydrogel technique accelerates the gelation reaction, structural qualities, mechanical properties, and cellular behaviors. Note that mechanical and biological qualities can be adjusted to reflect protein strengths. The shear storage modulus is designed to encompass soft-to-hard tissue matrix stiffness, ranging from 0.1 to 20 kPa along the iso-compositional line. Due to the mechanical synergism of both proteins' interpenetrating networks, silk fibroin/collagen hydrogels are highly elastic and resist permanent deformation under various stressors without collapsing or being water-squeezed out. The hybrid hydrogels' collagen protein component gives cells sticky sites, encouraging anchoring and spreading compared to mulberry silk fibroin gel, which lacks cell adhesion motifs. Silk fibroin/collagen hydrogels may enclose cells and maintain viability and proliferation in 3D culture. Our results show that silk/collagen hydrogels have adjustable and better physical and biological characteristics compared to protein gels, suggesting cell transport and tissue engineering applications.



## Increasing the Bioavailability and Preserving the Antioxidant Capacity of *Aronia melanocarpa* Extract by Encapsulation in Mesoporous Silica

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### Abstract

*Aronia melanocarpa* is considered one of the richest sources of antioxidants known, surpassing currants, cranberries, blueberries, elderberries, or gooseberries and contain one of the highest amounts of sorbitol. These plants are a rich source of vitamins, tocopherols, folic acid, and carotenoids. Fresh alcoholic extracts were loaded on mesoporous silica support (MCM-41) by the vacuum assisted method. We monitored the *in vitro* release of the loaded *A. melanocarpa* at two different pH values, by using simulated gastric fluid and simulated intestinal fluid. Additionally, *Staphylococcus aureus*, *Escherichia coli*, *Pseudomonas aeruginosa*, and *Candida albicans* were used to evaluate the antimicrobial activity of *A. melanocarpa* loaded mesoporous silica materials. In conclusion such functionalized mesoporous materials can be employed as controlled release systems for polyphenols or anthocyanins from natural sources.

### Acknowledgements

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## High Durability Virucidal Coatings Based on Microcapsulated Active Agents

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### Abstract

Transmission of pathogens through contaminated surfaces (fomites) is an important contributor to the spread of microorganisms as they possess the ability to survive on inanimate surfaces. A long lasting and passive antimicrobial surface using self-cleaning and self-sanitizing coatings can inhibit microbial transmission and prevent outbreaks. These antimicrobial surfaces interact with different pathogens via multiple active synergistic mechanisms. Although, several studies have shown promising results with virucidal/bactericidal properties, they seldom focus on the durability of the antimicrobial effect which has a limited life cycle. In this research, we have encapsulated a cytocompatible biocidal agent within porous polymer shells to create microcapsules with an average particle size of 40 - 50  $\mu\text{m}$ . These microencapsulated biocidal agents are incorporated into a polyurethane system to create highly durable thin films. Using this novel approach, composite coatings have been created that shows high efficacy against coronaviruses, e.g., CoV-OC43. Preliminary results demonstrate a 3log-reduction against OC43 for a period of 3 months. Investigations are ongoing to determine the release kinetics of the biocidal agents from encapsulated fillers using inductively coupled plasma optical emission spectroscopy. Studying the release kinetics will enable to fine-tune the concentration of biocidal agents and crosslinking chemistry of organic matrix to determine an optimal formulation for a long-lasting antiviral effect. This study will determine the life cycle of the composite coatings against OC43 that has not been previously reported for the proposed system. Surface characterization will be performed using a novel plasma etch X-ray photoelectron spectrometer for compositional depth profiling of the antimicrobial coatings.

## Future Hybrid Materials Based on CsPbX<sub>3</sub> Perovskites and Ce-UiO(66)-Y MOFs for Photocatalytic Applications

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### Abstract

Perovskites are characterized by a simple structure, strong light absorption (which is crucial in photocatalysis), controlled wavelength of light emission and simple synthesis process. However, despite many advantages, their low stability is a big problem. To solve it, CsPbX<sub>3</sub> perovskite particles were combined with the Ce-UiO(66)-Y MOFs during the ligand-assisted precipitation method to form novel nanohybrids. The obtained structures were used in the reaction of photocatalytic H<sub>2</sub> generation – effective production of H<sub>2</sub> and its use in place of highly emissive, harmful, non-renewable energy sources is a part of the activities leading to a low-emission economy.

### Acknowledgements

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## Pt/Perovskite/TNTs Photoanodes in Photoelectrocatalytic Processes

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<sup>3</sup>Advanced Materials Center, Gdansk University of Technology, Poland

### Abstract

Modified TiO<sub>2</sub> (titanium dioxide) is a widely used component for photocatalytic processes and, increasingly for photoelectrocatalytic processes. Therefore, the presented research includes the optimization of the anodic oxidation synthesis of TiO<sub>2</sub> nanotubes (TNTs) on technical titanium plates. The preparation of the samples was based on the previous achievements of our research team, but with minor changes. The effect of mixing, the type of electrolyte, the voltage of the electric current as well as the method of cleaning after the anodic oxidation process in terms of obtaining uniform nanotubes, were examined. Then, their surface was modified with perovskites containing rare earth metals (by spin coating method). The obtained samples (Pt/perovskite/TNTs) were tested in the processes of photo- and photoelectro-catalytic hydrogen generation, PEC CO<sub>2</sub> conversion and PEC degradation of phenol in aqueous solutions. The influence of modification of TNTs with different types of perovskites (LnFeO<sub>3</sub>, where Ln = Gd, Sm, Tm, Eu, and La) and irradiation with UV-Vis and Vis (> 420 nm) was investigated. The samples were characterized by DRS, XRD, SEM, and photoluminescence spectra.

### Acknowledgements

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## Carbon-based Composites with $\text{NaFeV}(\text{PO}_4)(\text{SO}_4)_2$ and $\text{Na}_4\text{Fe}_3(\text{PO}_4)_2\text{P}_2\text{O}_7$ for Improving their Electrochemical Performance

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### Abstract

Sodium transition metal phosphates have been attracting extensive attention as electrode materials for next generation cheaper metal-ion batteries for large scale application. The interest in these materials is determined by their high structural and thermal stability, safety, operation at higher temperatures and low cost, particularly for Fe-containing phosphates. However, the typical low conductivity resulting in low-capacity performance still restricts their practical application. One of the approaches to overcome this problem is to use composites with different high conductivity carbons as electrode materials. Here, we report on the electrochemical properties of carbon-based composites with two compounds having a tunnel-type structure and which compositions contain two kinds of anionic units:  $\text{NaFeV}(\text{PO}_4)(\text{SO}_4)_2$  and  $\text{Na}_4\text{Fe}_3(\text{PO}_4)_2\text{P}_2\text{O}_7$ . The composites are prepared with 15% carbon additives (reduced graphene oxide, rGO, and carbon black) via ball-milling treatment. The galvanostatic and potentiostatic experiments are conducted in Li-half cells at 25 and 40 °C. Charge-discharge performance and cycling stability are studied at C/2 rate. The effect of additives rGO and carbon black on the performance of  $\text{NaFeV}(\text{PO}_4)(\text{SO}_4)_2$  and  $\text{Na}_4\text{Fe}_3(\text{PO}_4)_2\text{P}_2\text{O}_7$  has been compared and analyzed based on electrochemical and physico-chemical data. The results demonstrate the effectiveness of carbon-based composites with sodium iron phosphates for improved electrochemical performance in hybrid metal-ion batteries.

### Acknowledgements

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## Development of Desalination Membrane Based on Ionic Hydrogel for Solar Vapor Generator System and their Salt Ion Activated Effect

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### Abstract

97% of the earth is surrounded by water, but the global water shortage is getting worse. Currently, membrane-based technologies such as reverse osmosis have been commercialized, but they have economic and regional differences in application. Therefore, to solve these limitations, research on solar desalination technology is being conducted. This is a technology that uses sunlight, an energy source freely available in most regions, to generate heat and produce fresh water. However, the problem of salt accumulation over time and deterioration of desalination performance due to this is still being raised. Therefore, in this study, we would like to suggest a way to solve the problems we are facing by using ionic hydrogels capable of interacting with salts on their own. First, we will discuss the results and reasons for various characteristics such as the change in water evaporation state due to the interaction of ionic materials with salt and the self-cleaning of salt crystals. Then, to evaluate the desalination performance, a membrane based on the synthesized ionic hydrogel material was prepared, which consists of a double-layer structure in which the conductive polymer PEDOT was introduced into the upper photo-thermal layer. The photo-thermal properties and evaporation rates of the prepared final membranes in simulated seawater of various concentrations were compared under 1 sun. Finally, it was possible to suggest additional ways to improve the desalination performance through the addition of pore in the same material, and the possibility of field applicability was confirmed by showing the highest value at a concentration of actual seawater.

## Bio-carbons as Sustainable Electrodes for Sodium-ion Batteries

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### Abstract

Searching for high-performance, low-cost, and sustainable electrode materials for sodium-ion batteries, bio-hard carbonaceous materials (bio-HCs) appear as an absolute favorite. The main drawbacks of bio-HCs are their critical dependence on the choice of the biomass precursors and the pyrolysis conditions. Therefore, the state-of-the-art research is directed to understand the relationships between synthetic conditions and electrochemical properties of bio-HCs.

Herein, we compare the Na-storage properties of bio-HCs derived from coffee grounds waste and walnut shell waste. For the preparation of bio-HCs, classical torrefaction and CO<sub>2</sub>-looping pyrolysis were used. The electrochemical properties of bio-HCs were analysed in model Na-ion cells with carbonate-based sodium electrolyte. The mechanism of Na-storage including capacitive and Faradaic reactions is evaluated by CV-experiments. To quantify the Na-storage performance of different bio-HCs, we determined four parameters: reversible specific capacity, first irreversible capacity, cycling stability and rate capability. Based on the above results, guidelines for selection of biomass as precursors for production of electrodes are proposed.

### Acknowledgements

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## Walnut Shell-derived Hard Carbons with Enhanced Na-storage Properties

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### Abstract

Hard carbons (HCs) are considered as the most promising anode materials for sodium-ion batteries (SIBs) due to their disordered pseudo-graphitic structures, large interlayer distance and nanovoids capable to insert the large sodium ions reversibly. In addition, HCs can be obtained from biomass, thus enabling to find a balance between high-power performance and sustainability of energy storage devices. The challenge is what type of biomass to be selected.

Herein we demonstrate the advantage of using walnut shell waste as a precursor for the preparation of HCs with improved Na-storage performance. HCs were prepared by two synthetic procedures including a classical torrefaction and hydro-pyrolysis. The impact of the synthetic procedures on the texture and Na-storage properties of HCs are examined in detail. The first irreversible capacity, the reversible specific capacity and rate capability of "walnut shell"-derived HCs are modified by variation in the co-pyrolysis procedures and additional acid treatment. The results obtained provide new perspectives for design of biomass-derived HCs as sustainable electrodes for SIBs.

### Acknowledgements

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## Heating Films Having the Characteristics of Positive Temperature Coefficient as well as Electromagnetic Wave Shielding Effectiveness Using Carbon-based Composite Paste

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### Abstract

Carbon microcoils (CMCs) were formed on stainless steel substrates using  $C_2H_2 + SF_6$  gas flows in a thermal chemical vapor deposition system. The incorporation of  $H_2$  gas into the  $C_2H_2 + SF_6$  gas flow system with cyclic  $SF_6$  gas flow caused the formation of the hybrid of carbon nanofibers-carbon microcoils (CNFs-CMCs). The electromagnetic wave shielding effectiveness of the heating film, made by the hybrids of CNFs-CMCs incorporated carbon paste film, was investigated across operating frequencies in the 1.5 - 40 GHz range. Although the electrical conductivity of the native commercial carbon paste was lowered by both the incorporation of the CMCs and the hybrids of CNFs-CMCs, the total SE values of the manufactured heating film increased following the incorporation of these materials. This dramatic improvement in the total SE values was mainly ascribed to the intrinsic characteristics of CMC and/or the hybrid of CNFs-CMCs contributing to the absorption shielding route of electromagnetic waves. Meanwhile, the heating film having the positive temperature coefficient thermo-electronic characteristics could be fabricated using the homemade carbon composite paste. The homemade carbon composite paste was composed of various kinds of carbon-based materials including the hybrids of CNFs-CMCs, graphene, and so forth. Almost 40% decrease of the output electric power in the heating film composed of the homemade carbon composite paste could be measured across from 30 °C to 80 °C. Finally, we could fabricate the commercial heating films which show the positive temperature coefficient thermo-electronic characteristics as well as the electromagnetic wave shielding effectiveness.

## Dielectric/ $TiN_xO_y$ Thin Films for Solar Driven Photoelectrochemical Water Splitting

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### Abstract

Photoelectrochemical (PEC) water splitting using sunlight has attracted much attention and regarded as one of the eco-friendly approaches for decades as it can convert solar energy directly into hydrogen. Several metal oxides have been used as photocatalytic materials, but due to their large band gaps their use is limited. As an alternative, surface plasmon polariton (SPP) between noble metal thin films and dielectrics was presented. Metal nitrides (TiN, ZrN, TaN, HfN, etc.) have metal properties in the visible light region. Especially TiN is a refractory material and cost-effective, TiN has attracted much attention as a candidate of noble metals. In order to improve SPPs performance of TiN,  $TiN_xO_y$  was used instead of TiN to control photocatalytic properties.  $TiN_xO_y$  films were fabricated via reactive RF-magnetron sputtering using Ar and  $N_2$  as reaction gases. Using X-ray absorption spectroscopy, SEM, and UV-Vis, the structural and optical properties of the films were analyzed. With increasing total gas pressure, the XAS analysis of  $TiN_xO_y$  films show Ti changed from  $Ti^{3.5+}$  toward  $Ti^{4+}$ , and decrease of long-range ordering. As substrate temperature increased, the oxidation state of Ti gradually increased, and structures approached finally to that of  $TiO_2$  brookite. ZnO was deposited as a dielectric material, and ZnO/ $TiN_xO_y$  films were fabricated, and PEC experiments were carried out to confirm their photocatalytic performance. Onset and plateau of the photocurrent were observed at low voltages, showing characteristics that were clearly different from those of ZnO films.

## Polymer Blends for Energy-efficient Construction Materials: Simulation Studies

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## Abstract

Phase change materials (PCM) represent a smart solution for improving energy efficiency in construction materials. PCM can store or release heat through a solid-liquid transition. When the transition temperature is in the human comfort zone (22 °C - 27 °C), PCM help to reduce energy consumption and dampen indoor temperature fluctuations. Pure PCM can leak from construction materials while they are in molten state. To avoid this, they can be macro and microencapsulated or dispersed in a medium that remains solid during the phase transition. The latter are termed shape-stabilized phase change materials (SSPCM). In the present work, we used molecular dynamics simulations to study the structure and compatibility of polyethylene (PE)/octadecane blends as models for SSPCM. Octadecane acts like PCM and PE prevents octadecane loss from construction materials. We studied blend miscibility as a function of PE concentration at two different temperatures, below and above the melting points of PE and octadecane. We applied Flory-Huggins theory to analyze the results, which showed a strong dependence on temperature. We also calculated mechanical properties of both concrete and gypsum containing PE/octadecane blends. We found that the incorporation of SSPM into these construction materials resulted in the degradation of their mechanical properties.

## Exploring the Properties of High Entropy Alloys for Hydrogen Storage

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### Abstract

In this research, four equimolar composite high-entropy alloys (CrMnFeCoNi (A1), AlCrFeCoNi (A2), CrMnCoNiCu (A3), and MnFeCoNiCu (A4)) were prepared using arc melting under an inert argon atmosphere. To ensure homogeneity, the samples underwent five remelting cycles, followed by grinding and sieving of the ingots. Powder samples ranging from 25 to 45 microns in size were utilized to investigate the phase compositions using X-ray diffraction. The results revealed that all HEAs (High entropy alloys), except A2, exhibited a single face-centered cubic phase (FCC), while A2 displayed the formation of a body-centered cubic phase (BCC). Notably, the BCC alloy demonstrated the lowest density and the highest hardness compared to the FCC alloys.

The microstructures of the synthesized materials were examined using a scanning electron microscope, and their chemical compositions were analyzed through energy-dispersive spectroscopy. Based on the findings, it appears that the investigated alloys hold potential as candidates for studying the processes of hydrogen absorption and desorption. The hydrogen storage properties of the HEAs will be evaluated and the obtained data will be presented for the first time at the forthcoming conference.

### Acknowledgements

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## Hydrogen Storage in Metal Hydrides

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### Abstract

The transition towards a sustainable and clean energy future requires the creation of advanced materials that can

effectively store and transport energy. Hydrogen has emerged as a favourable option due to its high density and eco-friendly characteristics. However, the key challenge lies in finding an efficient approach for storing and releasing hydrogen. Metal hydrides have gained substantial interest as potential materials for hydrogen storage because of their distinctive properties, including their ability to store large amounts of hydrogen, favourable thermodynamics, and potential for reversible uptake and release of hydrogen.

The selection of alloys was focused on alloys with the highest possible internal stress due to the presence and concentration of atoms with different atomic radii. These alloys exhibit a high degree of stresses at the atomic level but are still capable of forming a single-phase solid solution. In this work, we have investigated whether alloys in such a strained state have a higher ability to absorb and desorb hydrogen to and from their volume.

## Acknowledgements

This work was supported by the Slovak Research and Development Agency under the Contract no. APVV-21-0274 and APVV-20-0205. Authors are grateful to the Scientific Grant Agency of the Ministry of Education, Science, Research and Sport of the Slovak Republic and the Slovak Academy of Sciences VEGA project No. 2/0039/22. This research was funded in part by the international projects EIG CONCERT- Japan/2021/215 and M-ERA.NET 3/2022/235/H2MobilHydride.

## Redox Activity of New Peri-dichalogen Substituted Naphthalimides

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### Abstract

The study of oxidation-reduction reactions of organic materials dates to 1969, when the electrochemical properties of carbonyl compounds against Li-metal were studied. In 2008, Armand and Tarascon described the advantages of organic compounds with redox properties over inorganic ones and outlined their bright future. The highlighted organic materials have various electrochemically active groups such as imines, azo compounds, carbonyl compounds, organic radicals, etc. In recent years, scientific interest in organosulfur materials for rechargeable metal-ion batteries has grown exponentially.

Herein we present a combinatorial study for synergy between synthesizing *peri*-substituted dichalcogen naphthalimides and examining the reversibility of their redox reactions towards the alkali Li<sup>+</sup>/Na<sup>+</sup> ions. The redox properties of organosulfur materials were studied in Li- and Na-ion cells at room and elevated temperatures using carbon-based and ionic liquid-based electrolytes. It has been found that Li<sup>+</sup> and Na<sup>+</sup> ions interact with *peri*-substituted dichalcogen naphthalimides through reversible redox reactions that take place in a broad potential range.

### Acknowledgements

The financial support from the National Science Fund of Bulgaria (Project KP-06-H69/1) is acknowledged.

## Synthesis of 1,8-Naphthalimide Derivatives of Peri-substituted Dichalcogenides

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### Abstract

Herein we present the first part of a combinatorial study for synergy between the synthesis of *peri*-substituted

dichalcogen naphthalimides and the examination of the reversibility of their redox reactions towards the alkali ions  $\text{Li}^+$  and  $\text{Na}^+$ .

N-octyl-4,5-dibromo-1,8-naphthalimide was prepared from the imidization of 4,5-dibromo-1,8-naphthalic anhydride with 1-aminooctane, as we previously described in the literature. In parallel, we have prepared a novel 3,4,5,6-tetrachloro- and the 3,4,5,6-tetrabromo-1,8-naphthalic anhydride, which we could modify selectively at the peri-positions of the aromatic core. Dithiolo- and diselenolonaphthalimede were obtained in 91% and 88% yield, respectively, by treatment of N-octyl-4,5-dibromonaphthalene monoimide with S (or Se) in NMP at 170 °C for 6 h (8 h for Se). Similarly, the reaction of 3,4,5,6-tetrahalo-NMIs with S (or Se) in NMP at 170 °C for 4 h (6 h for Se) afforded the NMI-disulfide bridges compounds as well as the NMI-diselenide bridges compounds in 87 - 93% yield. NMR spectroscopic techniques, elemental analysis, mass spectrometry, and electrochemical tests have characterized the final compounds.

## Acknowledgements

The financial support from the National Science Fund of Bulgaria (Project КП-06-H69/1) is acknowledged.

## Ce-modified $\text{NaFePO}_4$ as Electrode Material for Sodium Ion Batteries

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### Abstract

The commercialization of the Na-ion batteries as cheaper alternative to Li-ion batteries is still a great challenge and one of the important issues is related to the choice of the most suitable electrode materials. Low cost per energy density, high safety, reliability, and sustainability are key requirements for the electrode materials. Among sodium intercalation compounds, the incorporation of a cheap and widely available redox element such as iron in the stable phosphate framework could largely meet the economic, safety and environmental requirements. The activation of both cationic and anionic redox reactions in the intercalation type electrodes is an effective way to double the energy density of lithium- and sodium-ion batteries. More recently, the use of oxygen storage materials such as  $\text{CeO}_2$  for stabilization of oxygen redox activity has been found to increase drastically the reversible capacity of  $\text{P3-Na}_{2/3}\text{Ni}_{1/2}\text{Mn}_{1/2}\text{O}_2$ . Moreover, first principle calculations have shown that anionic ( $\text{O}_2^-$ ) redox processes in  $\text{NaFePO}_4$  are also visible. Inspired by these data this study is focused on the Ce modified  $\text{NaFePO}_4$  as cathode material. To ensure a homogeneous Ce distribution, Ce acetate (2 and 5 wt.%) is introduced during the preparation of the phosphate precursor. The electrochemical performance of Ce-modified  $\text{NaFePO}_4$  is tested in galvanostatic and potentiostatic regimes in Na- and Li-half cells. The cycling stability and rate capability are studied at 20 and 40 C. Phase stability during the cycling is monitored by ex-situ techniques.

### Acknowledgements

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## 3D-Printing of Sugarcane-bagasse Ash-derived Zeolite Monoliths as Adsorbents

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## Abstract

There is an environmental concern over the impact related to increasing of CO<sub>2</sub> globally atmospheric concentration, the main greenhouse gas, which resulting in severe climatic change and pollution. These problems are directly related to high energy consumption from nonrenewable resources. To overcome this challenge, in this research work, sugarcane-bagasse ash (SBA) derived zeolite-porous monoliths with high affinity to CO<sub>2</sub> separation/capture were manufactured by 3D-printing, and the properties of this sustainable component were compared with that one produced using commercial zeolite 4A powder. Besides, 3D-printing technology has shown great potential to fabricate zeolite absorbents with hierarchical porosity and designed configuration through successive layer-deposition of optimized-inks containing bentonite (5 - 8 wt.%), methylcellulose (0.5 - 2.5 wt.%), and poly(ethylene glycol) (1 - 5 wt.%), as plasticizer, thickener and lubricant additives, respectively. The three-dimensional monoliths were freeze-dried at (-100 to -15 °C) for 1 h and then fired at 650 °C for 1 h at a heating rate of 10 °C/min. Afterward, the fired monoliths were transferred to a teflon capsule containing a mixture of 2.5 wt.% of Al(OH)<sub>3</sub> and NaOH 3 M solution and then, deposited into stainless steel autoclave at 80 °C (for 72 - 160 h) to provide the precipitation of zeolite crystals in situ. The SBA ash and synthesized zeolite A were then physically and chemically characterized. Preliminary results of Brunner-Emmet-Teller analysis for precipitated zeolite crystals after 160 h of hydrothermal treatment exhibited specific surface area of ~581 m<sup>2</sup>/g, in agreement with the data found in literature, indicating the viability of these zeolite monoliths use for CO<sub>2</sub> capture.

## Functional Materials Based on TiO<sub>2</sub> and Cs<sub>3</sub>Bi<sub>2</sub>X<sub>9</sub> for Photocatalytic Hydrogen Evolution

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### Abstract

One of the proposed materials is halide lead-free perovskites characterized by tunable bandgap, high efficiency, and ease of processing, making them an ideal candidate for photocatalytic hydrogen evolution. However, the main drawback is their long-term water and air stability. Therefore, to improve the chemical stability, charge transportation efficiency, and light absorption ability of perovskites, the materials consisting of Cs<sub>3</sub>Bi<sub>2</sub>X<sub>9</sub> (where X = Cl, Br, I) incorporated into TiO<sub>2</sub> nanoparticles were prepared. The experimental results and computational modeling enabled an understanding of the role of perovskite-type and loading in developing a highly efficient, non-toxic, and stable photocatalytic system.

### Acknowledgements

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## Carbon Nanotubes-metal Oxide Nanowire Networks for Energy-efficient Buildings

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### Abstract

Buildings in the European Union are the biggest energy consumers, responsible for 40% of energy usage and 36%

of CO<sub>2</sub> emissions. To cut energy consumption by up to 50%, thermal insulation is commonly used. To go further, in this work we propose incorporating thermoelectric modules in insulation panels to generate electricity from a temperature gradient of 10 - 30 °C, resulting in an additional 10% reduction in power consumption. Metal oxides like copper and zinc are cost-effective and eco-friendly for near-room temperature thermoelectric applications. However, their low electrical conductivity limits commercial use despite having a relatively high Seebeck coefficient.

Carbon nanotubes (CNTs) offer a solution by enhancing electrical conductance without significantly affecting the Seebeck coefficient. The study focuses on producing carbon nanotubes-zinc/copper oxide nanowire networks using various methods, such as chemical vapor deposition, annealing, thermal vacuum deposition, and thermal oxidation techniques. Electron microscopy, X-ray energy dispersive spectroscopy, and thermoelectrical measurements were used to characterize the networks.

The investigation revealed promising Seebeck coefficient and electrical conductance values, influenced by the proportion of CNTs and the quality of nanocontacts. Additionally, the study explored the impact of different binders on the properties of the metal oxide nanowire networks. This research highlights CNTs' potential to revolutionize energy efficiency in buildings.

## **Mach-Zehnder Interferometer with Distinct Layer Structures in Optical Isolator Employing Nonreciprocal Phase Shift**

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### **Abstract**

In optical communication systems, optical isolators are indispensable in protecting active photonic devices from unwanted reflected light. In the near infrared region, magnetic garnet crystals are necessary components of optical nonreciprocal devices because of their transparency and large magneto-optic coefficient. An optical isolator employing a nonreciprocal phase shift is attractive because there is no need for phase matching or complicated control of the direction of magnetization. The optical isolator consists of a Mach-Zehnder interferometer with nonreciprocal phase shifters in two arms. When the two arms in the interferometer have distinct layer structures, the device acts as an optical isolator operated with unidirectional external magnetic field.

In this paper, the author reports on the interferometric optical isolator employing the nonreciprocal phase shift. The magneto-optic waveguide has a magnetic-garnet guiding layer. The nonreciprocal phase shift is calculated for a various upper-cladding layer at a wavelength of 1.55 μm. The optical interferometers with an identical or a distinct layer structure are compared.

## **Enhancing the Conductivity of Copper Oxide Nanolayers by Alkali Metals**

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### **Abstract**

Wide bandgap inorganic materials (WBIMs) played a vital role in the development of modern semi-transparent technologies. WBIM based solar cells combining high transparency and good power conversion efficiency offer great opportunities for the BIPV sector. Copper(I) oxide which is a p-type intrinsic semiconductor with a wide band gap energy of 2.1 to 2.6 eV is a prospective material for this particular application. Cu<sub>2</sub>O is characterized by a high absorption coefficient in a visible range, a high chemical stability, a low price, and a non-toxic nature. Therefore, it has been studied extensively due to its applicability in optoelectronic devices, transparent electronics, or gas sensors [1]. However, the tricky method of single copper(I) oxide production and its high resistivity are main issues against



its commercial application. It should be mentioned that the resistivity of copper(I) oxide typically ranges from  $10^1$  -  $10^4$   $\Omega$ .cm for physical deposition methods and even  $10^6$   $\Omega$ .cm for chemical techniques [2]. Therefore, the biggest challenge is to find easy, cheap, and scalable deposition technique of copper(I) oxide, and to improve its electrical transport properties.

This work aimed to produce a low resistive copper(I) oxide nanolayer with calcium and potassium admixture by a simple spray coating technique. The used dopant precursors were calcium acetate and potassium acetate. It was found that calcium dopant reduced the resistivity of  $\text{Cu}_2\text{O}$  from 21  $\Omega$ .cm for as deposited copper oxide to 12  $\Omega$ .cm for doped thin films. While potassium admixture reduced it to even 5  $\Omega$ .cm. The phase composition as well as the optical, and electrical properties of manufactured oxides were studied. The photovoltaic properties of produced copper oxides were tested in n-i-p heterojunction with n-type Cz-Si. The I-V parameters were measured in STC conditions. The results confirmed that the tested alkali metals are effective admixtures to copper(I) oxide and that developed low resistive copper oxide can be a useful inorganic harvester for semi-transparent wide bandgap solar cell applications.

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## Ge-rich GeSbTe Phase Change Materials for Non-volatile Memory Applications in Flexible Electronics

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### Abstract

Non-volatile memories are a key requirement for the advancement of low-cost flexible integrated circuits (FlexICs), with potential future applications ranging from the Internet of Things to wearable electronics. Phase-change memories show promise for use in flexible electronics [1], and here we explore the use of Ge-rich compositions of GeSbTe (GST) in this application space. Ge-rich compositions offer the potential for higher crystallization temperatures when compared to the archetypal  $\text{Ge}_2\text{Sb}_2\text{Te}_5$  (GST-225) composition [2, 3], which, in addition to offering better data retention properties, means that the phase-change layer can remain amorphous during most manufacturing processes. This in turn means that a simple write-once memory format can be readily achieved, where only the relatively straightforward crystallization process is needed for memory operation. A write-once memory can then form the first stage in the development of a fully re-writable non-volatile device. In this work, therefore, we explore the use of Ge-rich GST compositions (specifically Ge content is  $\geq 50\%$ ) for both write-once and re-writable memories in flexible electronic formats. Various Ge-rich GST compositions were deposited and their fundamental properties, such as crystallization temperature and electrical conductivity, characterized. Memory devices on flexible substrates were also fabricated, and their switching characteristics investigated. Finally, the design and switching characteristics of GST memory cells suited to the FlexIC format were explored using finite-element and phase-change modeling.

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## Synthesis and Characterization of Environmentally Friendly Blue Emitting Quantum Dots with Functional Ligands

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### Abstract

Recent advancements in quantum dots have garnered attention as next-generation semiconductor nanomaterials due to their unique property of emitting light of different wavelengths depending on the size of the particles. However, quantum dots utilizing heavy metals such as Cd, Hg, and Pb face uncertainties in commercialization due to the European Union's RoHS (Restriction of Hazardous Substances Directive) regulations. As a result, research efforts are actively underway to develop environmentally friendly, green-emitting quantum dots, free from environmental concerns. Recently, ZnSeTe quantum dots have been developed by doping Te into ZnSe, thereby adjusting the bandgap, and achieving blue emission.

In this study, we synthesized ZnSeTe quantum dots with a multi-shell structure to enhance efficiency and stability while maintaining environmental friendliness. The blue emission of ZnSeTe was controlled by the degree of Te doping. Additionally, two functional ligands based on Dithiolane were introduced into the outermost shell to control the processability of the quantum dots, enabling both solubility and crosslinking capability. The synthesized quantum dots exhibited blue emission wavelengths suitable for display applications and demonstrated high color purity through PL and UV-Vis spectroscopic analysis.

Furthermore, the synthesis of functional organic ligands was confirmed through <sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F-NMR (Nuclear magnetic resonance) spectroscopy, and Fourier-transform infrared spectroscopy analysis. Ligand exchange was confirmed using <sup>1</sup>H-NMR and thermogravimetric analysis.

This study presents the successful synthesis and characterization of environmentally friendly blue-emitting quantum dots, showcasing their potential as promising candidates for future display technologies.

## Understanding the Role of Zn Vacancy Induced by Sulfhydryl Coordination for Photocatalytic CO<sub>2</sub> Reduction on ZnIn<sub>2</sub>S<sub>4</sub>

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### Abstract

How to regulate the energy barrier of \*COOH is the rate determining step of photocatalytic reduction CO<sub>2</sub> to produce gaseous CO. Herein, an appropriate Zn vacancy on ZnIn<sub>2</sub>S<sub>4</sub> was synthesized to achieve a desired photocatalytic CO<sub>2</sub> reduction capacity (CO: 5.63 mmol.g<sup>-1</sup>.h<sup>-1</sup>) and selectivity (CO: 97.9%). Various sulfhydryl group were selected to regulate the Zn vacancy formation in ZnIn<sub>2</sub>S<sub>4</sub>, which directly generated the unsaturated coordination state sulfur adjacent to Zn vacancy accompanied with less electron compared to ZnIn<sub>2</sub>S<sub>4</sub> without Zn vacancy. Comprehensive experimental analysis and theoretical calculations demonstrated that the appropriate Zn vacancy tuned the Gibbs free energy of \*COOH from the endothermic process to the exothermic process in the process of photoreduction

CO<sub>2</sub>. This work provided a cation vacancies engineering method for improving efficiency of photocatalytic CO<sub>2</sub> reduction by adjusting energy barrier of intermediate.

## Development of the Alcohol Reduction Method for the Designed Synthesis of Bimetallic Nanomaterials

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### Abstract

Bimetallic nanomaterials have attracted much attention from various fields such as catalysis, optics, magnetism, etc. The functionality of such particles is influenced very much by the intermetallic interactions rather than their individual contribution. However, compared with the synthesis of monometallic nanoparticles, the reaction parameters that need to be controlled for tuning the size, shape, composition, and crystal structure of bimetallic nanoparticles become challenging. This study focused on synthesizing bimetallic nanostructures using the alcohol reduction method where the control over the reducing power is conceivable by varying the combination of alcohol type, complexing agent, and metal salts. Consequently, various Cu-Co nanostructures such as Cu-Co core-shell, hollow alloy nanoparticles, and nanotubes were successfully synthesized by incorporating diffusion and etching phenomena during the reduction reaction. Moreover, time-resolved sampling revealed that the formation of Cu-Co alloy hollow nanostructure had been realized by the diffusion of the Cu core into the Co shell by controlling the reduction time gap between Cu and Co and the crystal structure besides the reduction sequences. It is noted that the synthesis of the high-temperature Cu-Co alloy phase was obtained at 170 °C. Among the Cu-Co alloy nanostructures, Cu-Co hollow alloy nanoparticles exhibited enhanced catalytic activity compared to metallic Cu and other Cu-Co nanostructures from the degradation reaction of methylene blue. The enhanced catalytic performance was considered mainly due to the alloy structure.

## Structural Properties of Single-walled Carbon Nanotubes Under Extreme Dynamic Pressures

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### Abstract

The structural behaviors of single-walled carbon nanotubes (SWCNTs) along the radial direction are critical to the cross-sectional phase transition, elastic recovery, and band structure engineering. Previous static pressure studies have established a clear picture on the structural behaviors of SWCNTs that governed by the Lévy-Carrier law. But when the pressurization becomes dynamic, there lack a fundamental understanding of the structural properties of SWCNTs along the radial direction. Here, different from static (< 1 GPa/s) and shock compression (> 10<sup>7</sup> GPa/s), we gain new insights on the phase transition, recovery dynamics and energy dissipation of SWCNT bundles with a median diameter of  $d_t \sim 1.4$  and  $\sim 0.8$  nm under modest dynamic pressures in two common pressure mediums (4:1 methanol-ethanol mixture, silicone oil). Upon single ramp compression (ramp rate in an order of magnitude of  $\sim 10 - 10^3$  GPa/s), the line shape and intensity changes of Raman spectra induced by the dynamic effect of hydrostatic stress are commonly observed, suggesting different structural behaviors compared with static pressure results. Unexpectedly, the pressure-induced defects are not found in cyclic ramp compressions up to 10<sup>5</sup> cycles, showing high structural stability to dynamic loading. The corresponding recovery dynamics and energy dissipation mechanism of SWCNTs under varying dynamic conditions are also discussed. By analyzing the shear strain potential, distinct dynamic effects of hydrostatic pressure on the SWCNTs in two pressure mediums are quantitatively unveiled.

## Effects of AlN Addition into AISI 316L on Microstructural Evolution During Laser Powder Bed Fusion

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### Abstract

316L stainless steel with the addition of 1 wt.% aluminum nitride (AlN) was manufactured by laser powder bed fusion, named 316L+AlN and compared with 316L manufactured using only 316L powder. AlN addition diminished the oxygen content from 468 ppm (316L) to 244 ppm (316L+AlN), but increased the nitrogen content from 842 ppm (316L) to 1293 ppm (316L+AlN). Reduction behavior was faster in 316L+AlN steel than in 316L steel. The addition of AlN changed not only the texture microstructure of steel but also nanoscale inclusions in the steel matrix. Epitaxial grains were larger in 316L+AlN steel than in 316L steel; this difference correlated well with the shape and temperature distribution of the melt pool. The inclusions in 316L+AlN steel were alumina, not nitride; this result means that nitride was supersaturated, while 316L had Si/Mn-rich oxide inclusions. Also, diminished oxygen content in 316L+AlN resulted in a decrease in the number density of inclusions and aluminum made the oxide inclusions larger. Supersaturated AlN in 316L+AlN could be precipitated in nanoscale with heat treatment. The yield strength was increased from 485.4 MPa to 583.2 MPa when 1 wt.% of AlN was added in 316L. 316L+AlN steel was stronger than 316L steel, primarily because of increased dislocation density in 316L+AlN steel.

## The Mechanical and Biological Characterisation of Avian Eggshell Membranes and Their Novel Application in Regenerative Medicine

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### Abstract

Chronic wounds affect millions of people annually and, in addition to the direct health implications, may also lead to significant mental, emotional, and financial distress. Current dressings often possess low biocompatibility, sub-standard mechanical characteristics, expensive to manufacture, and also suffer from ethical constraints. The eggshell membrane (ESM) is a naturally available and abundant material that has an innate complex structure and composition. With over 60 million tons of eggs produced globally per annum, utilization of this waste resource is highly attractive in view of sustainability. Although, the ESM has shown great potential as a novel biomaterial for wound dressing, a thicker and larger (i.e., surface area) membrane would offer greater opportunities for translational applications. As such, in this study, ESM samples were isolated from different avian species and characterised by FTIR, DSC, SEM and DMA with their properties reported in terms of thickness, optical transparency, porosity, wettability, fluid absorption, and mechanical characteristics. Cytotoxicity of the ESM samples was assessed *in vitro* using human dermal fibroblasts (ATCC, CRL-2522), and the angiogenic potential of the ESM determined by the chorioallantoic membrane (CAM) assay. Results indicated that all the ESM samples, regardless of species, exhibited similar values of cell proliferation level as the controls indicating high biocompatibility and pro-angiogenic properties. In addition, “Membrane-D” ESM showed similar physical properties to chicken ESM in terms of morphology and surface topography but displayed superior mechanical strength compared to that of chicken and “Membrane-R” samples. The high mechanical strength of “Membrane-D” ESM could be due to a lower porosity value observed. These findings suggest that species-specific ESM samples could be offered as a suitable alternative to bovine/porcine collagen as a wound dressing, yet also be modified to suit a range of biomedical applications.



## Three-dimensional Graphene TiO<sub>2</sub> Hybrids for Sunlight Driven Dye Removal

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### Abstract

The development of visible light-responsive photocatalysts has triggered significant interest due to their chemically green approach to effluent treatment. To this end, self-sustained macroporous hybrids of Three-dimensional (3D) graphene and titanium dioxide were synthesized, which exhibited excellent photodegradation performances of methyl orange, a highly resistant aromatic azo dye, under simulated sunlight. 3D graphene was grown on nickel foam by the thermal CVD method from a methane-hydrogen mixture and subsequently coated with a thin film of titanium dioxide employing either the sol-gel or the RF-sputtering method. Morphological and structural investigations indicate the formation of an interconnected, porous, and robust graphene network that replicates the shape of the nickel template. For the TiO<sub>2</sub> thin film, depending on the deposition method, it revealed the presence of an anatase phase in the case of sol-gel and an anatase-rutile mixture when deposited by RF-sputtering. The synthesized nanomaterials demonstrated an effective decolorization of methyl orange after exposure to simulated sunlight irradiation. The hybrid consisting of a pure anatase phase exhibited the most significant degradation efficiency of 94% after 30-min exposure to simulated sunlight, surpassing the performance of graphene alone (62.3%) or the hybrid containing a mixture of rutile and anatase phases (73.8%), making this hybrid an efficient sunlight-driven photocatalyst to decolorize the methyl orange azo dye. The degradation efficiencies of both hybrids increased above 95% after 90 min of sunlight exposure. Furthermore, the synthesized hybrid demonstrated similar degradation efficiency after three successive photodegradation cycles under simulated sunlight due to its foam-like structure and good mechanical stability.

## Valorization of *Ravenala madagascariensis* Leaves into Sustainable, High Performance Nanocrystalline Cellulose

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### Abstract

Nanocrystalline cellulose (NCC) is normally obtained from wood pulp but increasing attempts for non-wood sources such as sorghum, pineapple leaves and palm leaves have been reported. About 30% of nanocrystalline cellulose is derived from non-wood biomass. *Ravenala madagascariensis* is a resilient plant with a high leaf turnover and is largely underutilized. In this study, high quality cellulose from *R. madagascariensis* leaves was isolated and characterized. Cellulose extraction was done using a three-step procedure which involved soda pulping followed by two bleaching steps with sodium chlorite followed by hydrogen peroxide. The cellulose was repeatedly macerated at high speeds and filtered to remove larger cellulose. The NCC was dried in a convection oven at 70 °C to result in the translucent, white NCC sheet. The kappa number, cellulose, hemicellulose, lignin, and ash contents were determined. The cellulose was characterized using FTIR and SEM. The mechanical and optical properties were also investigated. A 33% yield of cellulose was obtained with 80% purity. FTIR revealed the absence of bands correlated with vibrations due to chemical bonds in lignin and SEM revealed that the fiber length ranged from 20 - 100 μm. The NCC sheets had burst strength and crease angle within acceptable ranges. Transmittance increased with decreasing particle size. This research provided a cost-effective, sustainable method for high quality NCC production from *R. madagascariensis*. It is anticipated that the NCC can be used in a variety of applications such as wastewater treatment, reinforcing materials, alternatives to plastics and circuits boards for nanotechnology applications.



## Investigation of the Biochemical Content of Individual Exosomes for Diagnostic and Therapeutic Purposes Using SERS

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### Abstract

Exosomes are extracellular vesicles of endosomal origin with lipid bilayer that are released by all types of cells. As a promising biomarker carrier for many diseases evidenced by recent research, exosomes encapsulate various biological molecules inherited from their parent cells as their cargo content, including miRNAs, mRNAs, and proteins. We aim to develop a technology for early population screening for cancer via exosomal liquid biopsy of the blood which is established on a per exosome basis with our unique SERS Identification of Molecules (SIM) platform. The information extracted from Raman spectra of exosomes will be subject to advanced data analysis using artificial intelligence, specifically, machine learning algorithms to help distinguish cancerous patients from healthy individuals as the diagnostic function. In addition, we are devoted to developing a monitoring technology for enhanced drug loading of exosomes for target-specific delivery with the SIM platform and understanding the factors influencing drug loading into exosomes from various perspectives, including loading uniformity and efficacy.

## Industry Talk

### FEA Materials: Aluminum Scandium Master Alloy Production Technology

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### Abstract

FEA Materials LLC (FEAM) has developed a hybrid metallothermic/electrolysis process (FEAM process) that enables production of Al-2%Sc below \$33/kg at scandium oxide market price of \$750/kg or lower. The FEAM Process can theoretically achieve Sc concentrations as high as 8 wt.% in the alloy, with consistent concentrations of up to 4 wt.% observed in experiments to-date. The system is designed for continuous operation and maintains a material yield above 90%. The FEAM process uses a proprietary molten salt composition that is both robust and self-correcting, overcoming the challenges with traditional electrolysis processes. The cell platform is modular, allowing for tuned production rates and flexible infrastructure requirements. The FEAM process runs under a controlled atmosphere to keep tight control of output streams and to ensure a safe work environment (no perfluorocarbon emissions). FEAM is currently producing upwards of 16 kg Al 2%Sc per shift with the capability to expand to 50 kg/shift within its facility in Westborough, Massachusetts.

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