

**2<sup>ND</sup> INTERNATIONAL CONGRESS ON**

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# **MATERIALS SCIENCE AND ENGINEERING**

**JULY 09-11, 2025**

**THE UNIVERSITY CARLOS III OF MADRID  
PUERTA DE TOLEDO CAMPUS MADRID  
SPAIN**

**ABSTRACT BOOK**

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## DAY – 1

### Keynote Talk

#### **In-situ investigation of nanomaterials with advanced electron probes**

*María Varela\*, Alejandra Guedeja-Marron, Francisco Fernandez-Cañizares, Gabriel Sanchez –Santolino, Rafael V. Ferreira, Juan I. Beltran, Neven Biskup, Lucas Pérez, Universidad Complutense de Madrid, Madrid, Spain.*

#### **Abstract:**

Our understanding of the properties of multifunctional nanomaterials relies on establishing the atomistic mechanisms responsible for functionality at the atomic scale. The success of aberration correction in the electron microscope has allowed electron probes to bear on this task with atomic resolution in real space, both in imaging and spectroscopy. Recent years have also witnessed the development of specimen holders that allow live materials to be tickled *in situ*. External stimuli, such as temperature or bias, can be used to modify systems of interest as we watch dynamics evolve, and this is a most important capability for nanomaterials. This talk will review examples of in-situ investigations of point defects in the scanning transmission electron microscope (STEM) in materials of interest for fields as diverse as spintronics or energy. An example can be found in the study of single Bi dopants in Cu nanowires with very low doping levels. These are very interesting systems due to the giant spin Hall effect associated with the presence of Bi. However, the dopant size and the presence of defects such as grain boundaries may promote Bi segregation when the temperature is raised or electric polarization is applied, which may affect the electrical performance of future devices based on these wires. Density-functional theory calculations show that for Bi doping levels below 1% the most stable dopant configuration is sitting within a Cu lattice site. Larger doping levels result in a distribution of different types of defects, being the substitutional ones the less prone to react to temperatures of a few hundred degrees C. Other point defects of interest in functional materials are vacancies. We will again combine theory, experiment and simulation to quantify and detect small concentrations of O vacancies in complex oxides. Simulations show that virtual detector optimization in 4D-STEM techniques can, in fact, lead to vacancy detection for vacancy compositions below 0.7%. Experiments including in-situ reduction processes will also be discussed.

#### **Biography:**

Maria Varela obtained her BS (1997) and PhD (2001) in Physics at the Complutense University, Madrid, Spain. She joined Oak Ridge National Laboratory as a Wigner Fellow in 2002 and was a Research Staff Member in the Materials Science and Technology Division until 2012. In 2010, she also became a Professor at Complutense University of Madrid (UCM) after being the recipient of an European Research Council Starting Investigator Award. Since 2023, she has been the director of the National Center for Electron Microscopy

at UCM. Her research experience includes thin film growth, transport properties, and structural characterization by electron microscopy, specializing in aberration-corrected scanning transmission electron microscopy and atomic resolution energy-loss spectroscopy. Her main research interests include a variety of topics related to magnetism and complex oxide nanosystems, thin films and superlattices, including high  $T_c$  superconductors, colossal magnetoresistance materials, multiferroics, dilute magnetic semiconductors, and other materials.

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## **Invited Talk**

### **Thermoplastic coatings on basalt fibers: a strategy to achieve interfacial Self-healing in composites**

Laura Simonini, Daniele Rigotti, Jeevan Kishore Reddy Pidapa, Alessandro Pegoretti <sup>1\*</sup>

<sup>1</sup>Department of Industrial Engineering, University of Trento, via Sommarive 9 – 38121 Trento, Italy

#### **Abstract:**

The aim of this work is to tailor the interfacial properties of fiber-reinforced composites to achieve interfacial self-healing by developing thermoplastic polymer coatings for basalt fibers using polycaprolactone (PCL) and poly(butylene adipate-co-terephthalate) (PBAT). The basalt fibers were coated with a fluid coating, with the thickness of PCL and PBAT controlled by the coating speed. Scanning electron microscopy revealed smooth and high-quality coatings at low coating speeds for both polymers. At higher coating speeds ( $> 20$  mm/s), PCL behaved like a Newtonian fluid, forming droplet-like structures. On the other hand, PBAT behaved like a non-Newtonian shear-thinning fluid, forming droplets at speeds above 80 mm/s. Contact angle measurements showed a significant reduction in contact angle hysteresis ( $\theta_H$ ) for fibers coated with both polymers compared to uncoated fibers, with PBAT exhibiting the lowest  $\theta_H$  and a smoother surface. The coated fibers were then combined with an epoxy matrix to form microcomposites and tested in a microdebonding configuration to measure the interfacial shear strength (IFSS). Moreover, the fiber/matrix interface was healed by a 30-minute thermal treatment at 80°C for PCL and at 120°C for PBAT, and a healing efficiency (HE) parameter was evaluated by repeating the microdebonding test. With the PCL PBAT coating, HE values up to 93.8% were obtained, very similar to the HE values of up to 89.5% achieved with the PBAT coating. In conclusion, both PCL and PBAT coatings proved to be effective in reaching interfacial healing in basalt fiber-reinforced epoxy composites.

#### **Biography:**

Alessandro Pegoretti is a Full Professor of Materials Science and Technology at the University of Trento (Italy). From 2012 to 2018, he was the Director of the Doctoral School in Materials, Mechatronics and System Engineering, and since 2021, he has been the Head of the Department of Industrial Engineering of the University of Trento. From 2022, Editor-in-

Chief of Polymer Composites, a journal of the Society of Plastics Engineers (SPE) devoted to reinforced plastics and polymer composites. He has authored over 330 refereed publications, 2 books, 15 book chapters, and 3 patents on various subjects in polymer and composites science and engineering.

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## Invited Talk

### **Spark Plasma Sintering of High- $T_C$ Sodium–Bismuth Titanate Ferroelectric Ceramics That Exhibit Superior Piezoelectric Performance**

*Chun-Ming Wang\*, Guo-Hao Li, Qian Wang, Fan Zhang, Yuan-Kai Yang, Heng-Tao  
School of Physics, Shandong University, Jinan 250100, Shandong, China.*

#### **Abstract:**

High-performance piezoelectric ceramics with excellent thermal stability are essential for high-temperature sensor applications. However, conventional fabrication methods offer limited improvements in piezoelectric performance. In this study, a significant enhancement in the piezoelectric performance of highly textured sodium–bismuth titanate ( $\text{Na}_{0.5}\text{Bi}_{4.5}\text{Ti}_4\text{O}_{15}$ , NBT) ceramics was achieved using the spark plasma sintering (SPS) method. The textured NBT ceramics exhibited a high degree of (00 $l$ ) orientation, with a Lotgering factor of 82%, a superior piezoelectric constant  $d_{33}$  of 35.8 pC/N, more than twice that of the ordinary sintered (OS) NBT (15.8 pC/N), and a high Curie temperature  $T_C$  of 661 °C. Microstructural analysis, domain characterization, and electrical property evaluation confirmed that polarization switching is more efficient in the textured ceramics, as demonstrated by scanning electron microscopy (SEM), piezoresponse force microscopy (PFM), and polarization–electric field ( $P$ – $E$ ) hysteresis loops. The direct-current (DC) resistivity of textured ceramics was significantly enhanced due to reduced bismuth volatilization and lower oxygen vacancy concentrations. Notably, the textured NBT ceramics exhibited outstanding thermal stability, with only a 17% variation in  $d_{33}$  from room temperature to 500 °C, while maintaining a high DC electrical resistivity of  $1.45 \times 10^6 \Omega \text{ cm}$  at 500 °C. This study not only underscores the potential of textured NBT ceramics for high-temperature piezoelectric sensors but also demonstrates an effective strategy for enhancing the piezoelectric properties of ceramic materials through spark plasma sintering.

#### **Biography:**

**Chun-Ming Wang** is a Professor in Physics at Shandong University, China. He earned his Ph.D. in Condensed Matter Physics there, rising from Assistant Professor to Associate Professor. After a two-year postdoc at the Australian National University, he became a Professor at Shandong University. He serves on key committees of the Chinese Physical Society and the National Technical Committee on Industrial Ceramics, and is Vice President of the Jinan Physical Society. As Associate Editor for the *Journal of the American Ceramic*

*Society* and other journals, his research focuses on dielectrics, piezoelectrics, ferroelectrics, photovoltaics, and their applications. He has over 160 publications and 10+ patents.

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## **Keynote Talk**

### **Advances in Curvilinear Magnetism: Cylindrical Magnetic Nanowires**

*Manuel Vazquez*

*Instituto de Ciencia de Materiales de Madrid, CSIC, Spain*

#### **Abstract:**

Curvilinear geometry in magnetic nanostructures (e.g., nanohelices, nanotubes, or rolled-up flexible multilayers) originates unprecedented phenomena whose manipulation leads to a new generation of technology applications. Particularly, cylindrical magnetic nanowires represent a novel 3D alternative (skyrmion tubes, magnetochiral-induced asymmetry, Bloch-point walls) to planar 2D systems whose most recent experimental advances are here reviewed. Nanowires (Fe, Co, Ni, and alloys, 20-400nm diameter) are synthesized by a controlled electrochemical route, a less-expensive technique allowing reliable systematic investigations. Their magnetization configurations reflect the energy balance between crystal anisotropy and stray fields. Particular interest is in engineered nanowires with modulations in diameter or composition leading to multilayered systems with axial, transverse, vortex, and more exotic magnetic configurations. Recent results in isolated nanowires have established their 3D magnetic character, conventionally taken as 1D. The reconstruction of 3D internal magnetic state is achieved by advanced microscopy techniques (e.g., Photo-Electron Emission and X-ray Transmission Electron Microscopies, with X-ray Magnetic Circular Dichroism), Vector-Field Electron Nanotomography, and Scanning Nitrogen-Vacancy Magnetometry, resolving local magnetic inhomogeneities. Remagnetization proceeds by Bloch-point walls and complex rotational processes where modulations induce controlled domain wall pinning and effects like magnetization ratchet. Under current pulses, walls are pushed to the nanowire end but re-nucleate under thermal fluctuations when the current is off. A wide spectrum of applications involving cylindrical nanowires is summarized: spintronics, robotics, magneto-thermoelectric effects, sensors, biomedical, and microwave absorption. -“Magnetic Nano-and Microwires”, M.Vazquez ed., Elsevier, 2020, ISBN: 9780081028322A.

#### **Biography:**

Manuel Vazquez is *Ad Honorem* Professor of Research, CSIC. Responsible for many scientific/technological projects on nano & microwires, he supervised 35 Ph.D. students, co-authoring 600 publications and 23 patents. Ph.D. by Complutense University of Madrid, postdoc at Max-Planck-Institute für Metallforschung (Humboldt) and Denmark Technical University, he was Laboratory Head at Institute of Applied Magnetism, IMA(1992-2000), Manager of the Spanish Strategic Action on Nanoscience and Nanotechnology(2004-09), and

funded the Nanomagnetism and Magnetization Processes Group, ICMM/CSIC (2001). He is an IEEE Life Senior member, founded the IEEE Magnetics Society Spain's Chapter, 2007, chaired the INTERMAG2008 conference, and was its President, 2017-18. He co-founded the Club Español de Magnetismo, 2002 and received the Salvador Velayos Magnetism Award, 2016.

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## Keynote Talk

### Features of hydrogels and composites for selective adsorption

*Alain Ponton<sup>1\*</sup>, E. Manso Castillo<sup>1</sup>, Williams Brett<sup>1</sup>, Imane Boucenna<sup>1</sup>, M.P. Mateo<sup>2</sup>, G. Nicolás<sup>2</sup>*

*<sup>1</sup> Laboratoire Matière et systèmes complexes (MSC), Université Paris Cité and CNRS, France; <sup>2</sup> Laboratorio de Aplicaciones Industriales del Láser, Universidade da Coruña, Spain*

#### Abstract:

The issue of environmental protection is of significant concern, and the remediation of polluted water has become a prominent area of research. This has led to the development and improvement of various methods for the degradation, coagulation, adsorption, or filtration of pollutants. Among these depollution methodologies, the efficient adsorption by using polymeric hydrogels and composites represents an intensively researched avenue. In this context, we have first optimised the elaboration of biopolymer hydrogels and studied their shear mechanical and structural properties. We subsequently demonstrated, by means of the laser-induced breakdown spectroscopy (LIBS) technique, that the adsorption of these hydrogels immersed in solutions containing metallic ions is a time-dependent process occurring either on the surface or in volume. Secondly, we synthesised graphene oxide platelet nanofillers, which we introduced into crosslinked hydrogels to elaborate hydrogel composites. The morphology and chemical structure of the graphene oxide nanofillers and composites were characterised using X-ray photoelectron spectroscopy and electron microscopy. For this purpose, images were analysed by a multilayer segmentation with a deep convolutional neural network. The rheological, swelling, and dye adsorption properties were then investigated as a function of the initial polymer and graphene oxide concentrations. The findings of this study demonstrate that the highest enhancements in viscoelastic and adsorption properties are achieved with a higher concentration of graphene oxide. A correlation between the swelling, adsorption, viscoelastic, and structural properties of the composites is proposed, thereby providing a more comprehensive understanding of graphene oxide-based hydrogels for dye adsorption.

## **Biography:**

Alain Ponton, who was awarded a Ph.D. in physics from Bordeaux University in France, has been appointed research director at the laboratory Matière et Systèmes Complexes (Université Paris Cité et Centre national de la recherche scientifique). His current research activities focus on understanding the links between the design and study of the thermo-mechanical and structural properties of complex materials at different spatio-temporal scales. In this regard, he combines expertise in soft matter physics, nanoparticle chemistry, and materials science. One primary research area is focused on magnetostimulable composites, whose properties can be modulated by the application of a magnetic field. A second area of research concerns the eco-responsible design of nanofiller-organic matrix composites for the selective absorption of molecules or pollutants, in particular composite hydrogels containing lamellar graphene oxide nanofillers or carbon dots.

He has published more than 70 papers in reputed journals and has participated in over 100 conferences. A part of his research activities on complex materials is carried out within international collaborations. He is also responsible for a Rheophysics and physical chemistry platform that provides a full range of experimental equipment and scientific expertise in the physical chemistry of dispersed media (particle dispersions, polymer solutions, gels, foams, composites) and the study of their structural properties by light scattering and optical microscopy, thermal properties by differential scanning microcalorimetry, and mechanical properties (shear, compression, elongation). In terms of his principal responsibilities, he was Vice-Dean valorization, elected member of the research committee and the academic council of the faculty of science (Université Paris Cité), group leader of the research team “Dynamics and Organization of Soft Matter” and member of the management committee of the laboratory Matière et systèmes complexes. He is now the Mission advisor for the High Council for the Evaluation of Research and Higher Education (Hceres).

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## **Invited Talk**

### **The influence of oxide layer formation on multimetallic materials on their catalytical performance**

*Piotr Zabinski\*, Dawid Kutyla, Katarzyna Skibinska*

*AGH University of Krakow, Al. Mickiewicza 30, 30-059 Krakow, Poland*

## **Abstract:**

Catalysts can be successfully prepared and modified by a simple electrochemical process. Their surface composition distinguishes catalytic activity toward hydrogen or oxygen evolution reactions. In this work, uniform metallic layers were synthesized using the one-step method from an electrolyte containing a crystal modifier. Electrodeposited layers were oxidized and/or reduced in the furnace at 100°C. The freshly electrodeposited coating was

stored in an air atmosphere for seven days. This results in an epitaxial oxide layer forming on the surface of the catalyst. Changes in the surface composition, confirmed by the XPS method, strongly influenced the wettability, catalytic performance, and size of evolved hydrogen bubbles. The conical Co-Ni surface with an epitaxial oxide layer formed in a controlled way possesses the best catalytic activity towards hydrogen and oxygen evolution. Conversely, the spontaneously formed oxide layer decreases the catalytic performance in the mentioned reactions compared with the fresh sample. That opens a possibility to control the electrocatalytic activity of the material by proper growth of a thin layer of oxides. The proper storage of synthesized samples is also essential due to their desired catalytic applications. Proposed controlled oxidation can be an accessible way to increase nanomaterials catalytic performance.

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## Keynote Talk

### **Functional materials for energy storage applications: extending lifetime and electrochemical performance**

*M.F. Montemor\**

*Centro de Química Estrutural, Institute of Molecular Sciences*

*Departamento de Engenharia Química, Instituto Superior Técnico, Universidade de Lisboa,  
Av. Rovisco Pais 1049 001 Lisboa, Portugal*

#### **Abstract:**

Electrochemical energy storage plays a pivotal role in Europe's efforts to transition to renewable energy and is crucial to meet the decarbonization targets. The lifetime and performance of devices are largely determined by the performance of their electroactive electrode materials. In recent years, this field has experienced intense research activity and notable technological advancements.

his field has seen significant research efforts, leading to notable advancements in recent years. However, despite the numerous solutions proposed, there remains a critical need for reliable approaches that utilize abundant, non-scarce materials and incorporate environmentally friendly electrolytes. This approach is necessary to implement a circular economy, fostering more sustainable energy storage solutions.

This presentation explores the latest progress in designing functional materials to improve electrochemical performance and extend the lifespan of two key technologies: asymmetric supercapacitors and electrolyzers. It covers the development and testing of novel electrode materials, including composite self-healing materials and recycled materials.

An overview of the most promising materials, particularly their long-term performance in aqueous electrolytes, will be provided, along with insights into the challenges and



opportunities for scaling up and commercializing these next-generation of energy storage devices.

Acknowledgments: The author would like to express her gratitude to all team members working on this topic. The author thanks Fundação para a Ciência e a Tecnologia (FCT, Portugal) for financial support under the project 2022.05187.

### **Biography:**

M.F. Montemor is a Full Professor at Instituto Superior Técnico, Department of Chemical Engineering.

Her scientific activity focuses on new functional coatings for surface protection and energy storage. She is a co-author of 20 book chapters and over 320 scientific papers. Her h-index is 76. She has been awarded the EFC medal and has received a Doctor Honoris Causa Degree from the University of Mons. Leading a scientific team of approximately 20 researchers, including PhD students, post-docs, and young researchers, she fosters a creative research environment conducive to cutting-edge research and innovation that addresses synergies between materials engineering research and industry needs. She is the co-founder of the company “Charge2C-NewCap,” which fabricates supercapacitors.

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### **Invited Talk**

#### **Cellulose nanocrystals functionalized with waste vegetable oils for sustainable applications in advanced materials**

*Loredana Maiuolo<sup>1\*</sup>, Antonio Jiritano<sup>1</sup>, Vincenzo Algieri<sup>2</sup>, Federica Meringolo<sup>1</sup>, Paola Costanzo<sup>1</sup>, Antonio De Nino<sup>1</sup>*

*<sup>1</sup> Department of Chemistry and Chemical Technologies, University of Calabria, Italy;<sup>2</sup> IRCCS NEUROMED - Istituto Neurologico Mediterraneo, Italy*

### **Abstract:**

In recent years, the research has focused attention on the realization and application of new sustainable and eco-friendly materials derived from renewable resources. Cellulose can be considered a versatile starting material with numerous advantages due to its biodegradability, biocompatibility, and remarkable mechanical properties. Among the various forms of cellulose, nanocrystalline cellulose (NCC) stands out for its high surface area, unique optical properties, and ability to be functionalized, making it an ideal candidate for advanced material applications. In this work, we describe the innovative functionalization of nanocrystalline cellulose with waste vegetable oils, WVO (i.e., sunflower oil), to realize a new eco-sustainable material with enhanced hydrophobic properties, providing a valuable method for recycling a common waste product. This synthesized material was also used to form composite materials at 1%, 3%, 5% and 10% w/w, with the commercial polymer

Ecovio®. The new composite material was filmed using the solvent casting method. Finally, the effects of this additive on the mechanical properties of the final material were evaluated.

### **Biography:**

Loredana Maiuolo is an associate professor of Organic Chemistry at the University of Calabria, Italy. She is the principal author or co-author of over 100 scientific papers and a member of numerous financed projects, including the PRIN 2022 project "SOTERIA" PNRR M4.C2.1.1.2022WZK874. Her main research topics include: 1) Preparation of composite biomaterials useful in the Environmental, Automotive, Building, and Food Packaging sectors. 2) Preparation of composite materials with high mechanical resistance. 3) Organic synthesis of molecules of biological interest in eco-friendly conditions. 4) Preparation of Nanoparticles and their applications.

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### **Invited Talk**

#### **Computer simulation aspects of nanoparticle and nanodevice design**

*Panagiotis Grammatikopoulos<sup>1\*</sup>*

*Instituto Regional de Investigación Científica Aplicada (IRICA) and Departamento de Física,  
Universidad de Castilla-La Mancha, 13071, Ciudad Real, Spain*

### **Abstract:**

Cluster beam deposition (CBD) is a term that collectively describes various physical methods of nanoparticle synthesis by nucleation and growth from a supersaturated atomic vapour. It provides a solvent- and effluent-free method to design monodisperse multifunctional nanoparticles with tailored characteristics that can be subsequently deposited on a desired substrate or device in the soft-landing regime under ultra-high vacuum.

In this talk, I will explain the main mechanisms that control the basic properties of individual nanoparticles such as size, shape, or chemical ordering, based on various setups of CBD sources. Moving to a coarser scale, I will bring up examples where larger structures can be designed using nanoparticles as their functional building blocks, such as novel sensors and energy storage devices.

To date, CBD faces two main limitations that need to be overcome for real-world applications: (i) limited yield, and (ii) precise structural control. The main thesis of this talk is that both challenges can be tackled by in-depth theoretical understanding of both the thermodynamics and kinetics of nucleation & growth. To this end, atomistic computer modelling can be an invaluable tool, complementing experimental fabrication and guiding future source design.<sup>1</sup>

[1] P. Grammatikopoulos, *Current Opinion in Chemical Engineering*, **2019**, 23, 164.

## Biography:

Panagiotis Grammatikopoulos is a computational nanotechnologist. His research focuses on fundamental processes regarding nanoparticles but extends to device fabrication and applications. Panagiotis did his PhD at the University of Liverpool, UK. He has worked as a Research Associate for NCSR Demokritos, Greece, and the University of Greenwich, UK, and as Group Leader at OIST, Japan. Since 2020, he has been a Visiting Assistant Professor at ETH Zürich, Switzerland, a Specially Appointed Assistant Professor at Osaka University, Japan, and an Associate Professor at GTIIT, China. Panagiotis is currently Professor Distinguido “Beatriz Galindo” at UCLM, Spain.

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## Invited Talk

### Unusual Properties of Interlocked Metal Organic Nanocages

*Antonino Famulari, Javier Martí-Rujas*

<sup>1</sup>*Dipartimento di Chimica Materiali e Ingegneria Chimica “Giulio Natta”, Politecnico di Milano, Milan, Italy.* <sup>2</sup>*INSTM Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali.* <sup>3</sup>*Center for Nano Science and Technology@Polimi, Istituto Italiano di Tecnologia, Milan, Italy*

*[Note: Please use the font “Calibri 12”, unless specified]*

## Abstract:

In this contribution, some of the features of poly-[n]-catenanes composed of interlocked  $M_{12}L_8$  icosahedral nanometric cages are presented as obtained by the combination of X-ray diffraction experiments and Quantum Chemical (QC) calculations [1]. The TPB (exotridentate trispyridyl benzene) ligand and  $ZnX_2$  (with  $X=F, Cl, Br, I$ ), in the presence of appropriate templating solvent molecules, form metal–organic nanocages, microcrystalline materials. Single-crystal X-ray data allowed to solve the structure to be solved and to detect guest molecules exchange together with crystal-to-crystal phase transitions. The processes of crystallization, guest absorption, and release are driven by intramolecular and intermolecular interactions. QC calculations [2] were used to rationalize the observed physical process. Key factors in the formation of the poly-[n]-catenane and in solvent exchange mechanisms are modeled by a hierarchical mechanism of “closed-open” dynamic channels. The labile nature of the Zn–N coordination bonds allows the recyclability of the TPB ligand in water, thus making these materials very good candidates in green chemistry applications.

[1] a) S. Torresi, S. Famulari, and J. Martí-Rujas, *J. Am. Chem. Soc.*, 2020, *142*, 9537. (b) J. Martí-Rujas, S. Elli, A. Famulari, *Sci. Rep.* 2023, *13*, 5605. (c) S. Elli, A. Famulari and J. Martí-Rujas, *ChemPlusChem* 2024, *89*, e202400332.

[2] a) A. Famulari, G. Raos, A. Baggioli, M. Casalegno, R. Po, S. V. Meille, A solid state Density Functional study of crystalline thiophene-based oligomers and polymers. *J. Phys.*

*Chem. B*, 2012, *116*, 14504-14509; b) J. Martí-Rujas, S. Ma and A. Famulari, *Inorg. Chem*, 2022, *61*, 10863-10871.

## Biography:

Antonino Famulari graduated (1994) and completed his PhD in Chemistry (1998) at the Università degli Studi di Milano. In 2000, he was appointed to a Permanent Research position by the CNR center ISTM (Scienze e Tecnologie Molecolari) of Milan, and in 2001 he moved as an Assistant Professor to the Dipartimento di Chimica, Materiali e Ingegneria Chimica “Giulio Natta” of the Politecnico di Milano (Associate Professor since 2014). Currently, he is working on Molecular Modeling and X-ray scattering methodologies. Main research interests: a) structure and morphology of molecules (including oligomers and polymers) and di-metal organic frameworks (MOFs) and of composites and nanocomposites; b) intermolecular interactions; c) study of new devices for low-cost and environmentally impact production of oxides, hydroxides, and carbonates. He is the author of more than 120 scientific papers (3300 citations, H-index 33, June 2025), 3 patents, and more than 60 communications to international conferences.

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## Invited Talk

### Anisotropy and distribution of exchange interactions in Fe<sub>80</sub>B<sub>20</sub> thin films: the role of PLD Ar pressure

*Jimena Soler-Moralaa,\*, Rubén Fernández-Jiménezab, Verónica Brazac, Luis Vázquez, Daniel F. Reyesc, Sergio Jiménez-Fernándezd, David Gonzálezc, Juan Rubio-Zuazo, Jesús M. González and F. Javier Palomaresa*

*a*Instituto de Ciencia de Materiales de Madrid – CSIC, 28049 Madrid, Spain

*b*Escuela de Doctorado, Universidad Autónoma de Madrid, 28049, Spain

*c*IMEYMAT – Universidad de Cádiz, 11510 Puerto Real, Cádiz, Spain

*d*BM25-SpLine Beamline at the ESRF, 38043 Grenoble, France

## Abstract:

Amorphous metal-metalloid thin films have emerged as a promising class of materials for advanced magnetic applications [1]. Their unique combination of magnetic properties —such as low coercivity, high saturation magnetization, and highly tunable anisotropy [2, 3] — underlines their potential for integration in high-frequency electronics, novel spintronic devices, and a wide range of sensors [1].

In this work, we report on the chemical, structural, and morphological modifications introduced in nanothick Fe<sub>80</sub>B<sub>20</sub> films by the use of Ar assistance (at different pressures) during their pulsed laser ablation deposition process. The morphology and stoichiometry of the samples were characterized using X-ray photoelectron spectroscopy (XPS) depth profiling, atomic force microscopy (AFM), and high-resolution transmission electron

microscopy (HR-TEM). The magnetic behaviour was further studied through the angular dependence of dc hysteresis loops, high-field magnetization measurements, and dynamic response in the tens of GHz range.

The results show that when Ar-assisted deposition is used, partial crystallization occurs, leading to the formation of Fe-rich columns whose lateral dimensions increase with increasing Ar pressure. This same increase in Ar pressure also induces greater surface roughness and promotes a more isotropic in-plane magnetic hysteresis. Moreover, samples deposited at higher Ar pressures exhibit a spin wave stiffness constant nearly twenty times larger than that of the reference sample. Interestingly, the ferromagnetic resonance damping parameter is reduced in comparison to the reference, suggesting an enhancement in the dynamic magnetic performance by Ar assistance during growth.

[1] S. Bhatti, R. Sbiaa, A. Hirohata, H. Ohno, S. Fukami, S.N. Piramanayagam, *Spintronics-based random access memory: a review*, Materials Today 20 (2017) 530–548.

<https://doi.org/10.1016/j.mattod.2017.07.007>.

[2] A.L. Greer, *Metallic glasses on the threshold*, Materials Today 12 (2009) 14–22.

[https://doi.org/10.1016/S1369-7021\(09\)70037-9](https://doi.org/10.1016/S1369-7021(09)70037-9).

[3] G. Herzer, *Modern soft magnets: Amorphous and nanocrystalline materials*, Acta Mater 61 (2013) 718–734. <https://doi.org/10.1016/j.actamat.2012.10.040>.

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## Invited Talk

### **Metallic nitride multilayers for bipolar plates of proton exchange membrane water electrolyzers**

Carlos Prieto<sup>1,4</sup>, Eva Céspedes<sup>1</sup>, Alicia de Andrés<sup>1,4</sup>, María Retuerto<sup>2</sup>, Sergio Rojas<sup>2</sup>, Esteban Climent-Pascual<sup>3,4</sup>

<sup>1</sup> Instituto de Ciencia de Materiales de Madrid (ICMM), Consejo Superior de Investigaciones Científicas, 29049 – Madrid (Spain).

<sup>2</sup> Instituto de Catálisis y Petroleoquímica, Consejo Superior de Investigaciones Científicas, 29049 – Madrid (Spain).

<sup>3</sup> Departamento de Ingeniería Química y Medio Ambiente, Escuela Técnica Superior de Ingenieros Industriales, Universidad Politécnica de Madrid, C/José Gutiérrez Abascal 2, 28006 – Madrid (Spain).

<sup>4</sup> 2D-nanomaterials for Energy & Sensors applications, Univ. Politécnica de Madrid, Unidad Asociada Consejo Superior de Investigaciones Científicas (Spain).

#### **Abstract:**

Thin ZrN and TiN coatings are being investigated for use on stainless steel in bipolar plates of proton exchange membrane water electrolyzers. Reactive sputter deposition parameters, such as base vacuum pressure, N<sub>2</sub>/Ar ratio, and working sputtering pressure or magnetron supplied power, have been explored to obtain films optimized for electrical conductivity. Following optimization and microscopic characterization of its properties, the

electrochemical behavior of stainless steel coated with different films has been evaluated. The corrosion current density obtained for a ZrN/TiN/ZrN trilayer on AISI-304 supermirror stainless steel demonstrates its potential as an electrode on bipolar plates of proton exchange membrane water electrolyzers.

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## Day 2 – Room A

### Invited Talk

#### **Bilayer magnetic composite systems made of Few-Layer Graphene and Amorphous Magnetic Microwires for stealth technology**

*P. Marina,<sup>a,b</sup>*

*a Instituto de Magnetismo Aplicado. Universidad Complutense de Madrid –ADIF, AV km 22,5 28230 Las Rozas, Spain*

*bDepartamento de Física de Materiales. Universidad Complutense de Madrid. Pza de las Ciencias 1, 28040 Madrid, Spain*

#### **Abstract:**

This study explores the fabrication and application of two advanced materials for microwave absorption: defective few-layered graphene mesostructured (DFLGMs) and amorphous  $\text{Fe}_{73.5}\text{Si}_{13.5}\text{B}_9\text{Cu}_1\text{Nb}_3$  microwires (MWs).

DFLGMs are synthesized from graphite flakes through high-energy milling, allowing precise control over their structural features and defect generation. When combined with MWs in a paint matrix, the resulting composite exhibits notable improvements in microwave absorption, including a 47% reduction in the minimum reflection loss coefficient ( $\text{RL}_{\min}$ ) and a 137% increase in effective absorption bandwidth (EAB). These results demonstrate tunable absorption behavior and validate the applicability of the Maxwell-Garnett effective medium model for microwave attenuation [1].

The second material, MWs, undergoes a refinement process to control their length, resulting in homogeneous microstructures. These microwires exhibit both soft magnetic behavior and microwave absorbing capabilities. When incorporated into commercial paints and applied onto metallic substrates, coatings achieve reflection loss values approaching -40 dB within specific frequency ranges. By adjusting MW length, precise tuning of  $\text{RL}_{\min}$  within the GHz range is possible, making these composites suitable for frequency-selective absorption. Experimental and theoretical results show strong agreement, confirming the potential of these materials for tailored microwave absorption applications with low filler content and high attenuation performance [2].

[1] J. López-Sánchez, A. Peña, A. Serrano, A. del Campo, O. Rodríguez de la Fuente, N. Carmona, D. Matatagui, M. C. Horrillo, J. Rubio-Zuazo, E. Navarro, P. Marín, *ACS Appl. Mater. Interfaces* 2023, 15, 2, 3507–3521 (2023)

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## Invited Talk

### Design, screening and characterization of microfluidic-synthesized lipid nanocarriers: a synchrotron study

*Ilaria Clemente\*<sup>1,2</sup>, Giulia Gabbricci<sup>1,2</sup>, Luigi Talarico<sup>1,2</sup>, Gemma Leone<sup>1,2</sup>, Agnese Magnani<sup>1,2</sup>*

*<sup>1</sup> University of Siena, Department of Biotechnology, Chemistry and Pharmacy, Siena, Italy*

*<sup>2</sup> Center for Colloid and Surface Science (CSGI), Siena Research Unit, Florence, Italy]*

#### **Abstract:**

In the past decade, lipid-based nanocarriers have gained increasing popularity as an emergent technology for drug delivery. Since their approval for clinical usage, several lipid nanocarrier formulations have been investigated to obtain optimal physicochemical properties and enhanced therapeutic efficacy. Among the factors influencing structure, stability, and cellular uptake, the choice of lipid components plays a major role. Generally, the main constituents are helper or structural lipids (i.e., phospholipids and cholesterol), which provide stability and membrane fusogenicity. Then, either ionizable lipids for lipid nanoparticles (LNPs) or solid lipids for solid LNPs (SLNs) respectively, are employed to improve cargo encapsulation and protection from leakage. Finally, surfactant or polyethylene glycol-lipid coatings enhance in vivo circulation time. Thus, manipulation of composition and relative abundance results in dramatic modification of physicochemical properties. Microfluidic-assisted preparation of lipid nanocarriers allows for the obtaining of monodisperse and stable formulations with high reproducibility, boosting screening and optimization potential. In this work, high-throughput screening and optimization of three types of lipid nanocarriers, i.e., LNPs, SLNs, and transethosomes as candidates for drug delivery, is proposed. Microfluidic synthesis allowed for screening a large set of lipid components, surface coatings, and relative compositions following an experimental design approach. Supramolecular characterization by means of Dynamic Light Scattering, Zeta potential, Small Angle X-ray Scattering, and quantification of encapsulation efficiency of model drugs by High Performance Liquid Chromatography allowed to selection of the optimal carrier candidates.

Authors acknowledge funding from NextGenerationEU, PNRR M4C2, ECS00000017, CUP B63C22000680 007.

#### **Biography:**

Dr. Ilaria Clemente is an Assistant Professor at the Department of Biotechnology, Chemistry, and Pharmacy of the University of Siena, Italy, where she teaches a course in the Chemistry Master's degree titled "Smart Materials and Nanocarriers". In 2022, she defended her PhD in Chemical and Pharmaceutical Sciences, focused on the development, synthesis, and advanced physicochemical characterization of soft matter nanosystems for drug delivery purposes. Her main expertise and background involve soft matter chemistry, nanosystems and materials characterization, scattering techniques (i.e., Dynamic Light Scattering, Small/Wide Angle X-



ray and Neutron Scattering), Electron Microscopy (Transmission and Scanning Electron Microscopy), and microfluidic preparation.

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## Invited Talk

### Excellent piezoelectric properties and electrical resistivity of bismuth titanate-ferrite

*Qian Wang<sup>1\*</sup> and Chun-Ming Wang<sup>1,2</sup>*

*<sup>1</sup> School of Physics, State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100, China; <sup>2</sup> Center for Optics Research and Engineering (CORE), Key Laboratory of Laser and Infrared System of Ministry of Education, Shandong University, Qingdao 266237, China*

#### Abstract:

The development of high temperature piezoelectric sensors requires high performance piezoelectric materials with high Curie temperatures. The Aurivillius-type bismuth titanate-ferrite  $\text{Bi}_5\text{Ti}_3\text{FeO}_{15}$  has promising potential for high-temperature piezoelectric applications because of the high Curie temperature  $T_C$  ( $\sim 761^\circ\text{C}$ ). However, the high-temperature piezoelectric properties of  $\text{Bi}_5\text{Ti}_3\text{FeO}_{15}$  have not been sufficiently studied yet. By compositions adjusting, the high-temperature piezoelectric performances of the lanthanide or transition metal elements substituted  $\text{Bi}_5\text{Ti}_3\text{FeO}_{15}$  were studied. The intrinsic and extrinsic contributions to the enhancement of piezoelectric properties of the substituted  $\text{Bi}_5\text{Ti}_3\text{FeO}_{15}$  were investigated in detail. As a result, the substituted  $\text{Bi}_5\text{Ti}_3\text{FeO}_{15}$  compounds exhibit high piezoelectric constant  $d_{33}$ , which is three times larger than that of the unsubstituted  $\text{Bi}_5\text{Ti}_3\text{FeO}_{15}$ , together with high  $T_C$  of  $>750^\circ\text{C}$ . These results suggest that the substituted  $\text{Bi}_5\text{Ti}_3\text{FeO}_{15}$  compounds are potential candidates for high-temperature piezoelectric applications

#### Biography:

Qian Wang, is currently an assistant professor at the School of Physics, Shandong University. She obtained her PhD degree from the School of Physics, Shandong University, in 2020. She has been engaged in the preparation and research of high-temperature piezoelectric materials and devices. She holds 2 patents and has published 30+ papers in *J. Euro. Ceram. Soc.* and *J. Am. Ceram. Soc.*, etc., with SCI citations  $>550$  and h-index of 13. She was awarded “Rising Star” by the American Ceramic Society in 2024.

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## Invited Talk

### Expanding Horizons of Metal–Phenolic Networks by tailoring Electrochemical Strategies

*Maddalena Corsini<sup>1\*</sup>, Andrea Atrei<sup>1</sup>, Fabrizia Fabrizi de Biani<sup>1</sup>, Giuseppe di Florio<sup>2</sup>*

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*<sup>2</sup> ENEA, Italy*

#### Abstract:

Nature is a great source of inspiration by virtue of millions of engineered and crafted processes and materials. Inspired by nature, a new class of materials is emerging: metal–phenolic networks (MPNs). MPNs are hybrid composite materials with broad potential across biomedicine, energy, and materials science. [1] Composed of polyphenols and metal ions, they exhibit strong and tunable adhesion properties governed by catechol chemistry, similar to the mechanism mussels use to adhere to surfaces. Leveraging these interactions, MPNs can self-assemble into functional coatings with tailored physicochemical properties. Among various fabrication strategies, electrochemical deposition offers a powerful and controllable approach for MPN film growth. This method exploits the redox activity of polyphenolic ligands and metal ions to promote rapid film formation on conductive substrates under mild, aqueous conditions. In this work, we explore electrotriggered MPN assembly using pyrogallol in the presence of Fe(III) ions. The resulting coatings were characterized by AFM, SEM, EDX, and UV-vis spectroscopy. Particular focus is given to AFM, which provides nanoscale insight into surface morphology and reveals key aspects of the film growth mechanism. Furthermore, persistent homology, a tool in materials informatics for analyzing multiscale topological features [2] is applied to AFM data to track MPN film evolution during electrodeposition. Overall, this assembly technique demonstrates the potential of electrochemical methods for the controlled fabrication of functional MPN materials.

#### Biography:

[1]. F. Caruso *et al.*, Metal-Phenolic Network composite: from fundamentals to applications, *Chem. Soc. Rev.*, 2024, 53, 10793-10793

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## Invited Talk

### Bioactive Metal Complexes With Thiourea Derivatives

*Aleksandra Drzewiecka-Antonik<sup>1</sup>\*, Anna Wolska<sup>1</sup>, Paweł Rejmak<sup>1</sup>, and Marcin Klepka<sup>1</sup>*

*<sup>1</sup>Institute of Physics, Polish Academy of Sciences, 02-668 Warsaw, Poland*

#### Abstract:

Metal complexes with thiourea derivatives have emerged as promising candidates for the development of antibacterial and anticancer drugs. The cytotoxic properties of such complexes are often enhanced compared to the metal ion or the ligand alone. Thioureas are versatile ligands that can be easily modified to change the properties of complex, leading to improved targeting of bacterial/cancer cells and reduced toxicity to healthy tissues. This fact prompted us to start the synthesis of new compounds based on *N,N*-disubstituted thiourea derivatives. We have designed and investigated copper and platinum complexes containing a thiourea moiety [1-5]. To analyze the influence of the structure of new compounds on their bioactivity, the structural characterization of amorphous complexes was carried out. For this purpose, the compounds were studied using ATR-IR, UV-Vis, and EPR spectroscopy. Moreover, a methodology based on X-ray absorption fine structure spectroscopy (XAFS) using synchrotron radiation was employed [6]. The results obtained from the extended X-ray absorption fine structure (EXAFS) analysis, combined with density functional theory (DFT) and X-ray absorption near edge structure (XANES) calculations, allowed us to propose a 3D molecular structure of the new complexes. Through further changes in the structure of the starting ligand, we aim to obtain the complexes with the desired biological activity.

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- [2] J. Inorg. Biochem. 212 (2020) 111234;
- [3] Int. J. Mol. Sci. 22 (2021) 11415;
- [4] Int. J. Mol. Sci. 23 (2022) 15694;
- [5] Synchrotron Radiation In Natural Science 25 (2025) 64;
- [6] Chem. Phys. Lett. 691 (2018) 190.

#### Biography:

Dr. Aleksandra Drzewiecka-Antonik is an assistant professor at the Institute of Physics of the Polish Academy of Sciences in Warsaw, Poland. She deals with the synthesis and structural analysis of bioactive metal complexes with organic ligands. In her work, she uses the following research techniques: IR, UV-Vis, XRD, EXAFS, XANES.

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## Invited Talk

### Methods of High Entropy Alloys oxidation

*Katarzyna Skibińska<sup>1\*</sup>, Dawid Kutyla<sup>1</sup>, Mateusz M. Marzec<sup>2</sup>, Piotr Bala<sup>3</sup>, and Piotr Żabiński<sup>1</sup>*

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#### **Abstract:**

High-Entropy Materials (HEMs), including High-Entropy Alloys (HEAs), High-Entropy Oxides (HEOs), and other High-Entropy Compounds, are gaining significant interest. HEAs are a class of metallic materials typically containing five or more primary elements in near-equal atomic concentrations ranging from 5 to 35 at. % (2-3). They show unusual mechanical properties, corrosion resistance, thermal stability, and magnetic properties, which make them suitable candidates as catalysts for water splitting, hydrogen storage material, as well as electrodes in batteries for charge storage in supercapacitors. HEAs and HEOs share similar structural features since they both contain more than 5 elements, usually metals, while HEOs contain 5 or more cations and an oxygen sublattice. HEOs show a wider variety of crystal structures and local site symmetries. Their optical and magnetic properties can be utilized in energy storage and catalysis.

Various oxidation methods were applied. The chemical and structural properties of the produced samples were analyzed using XRD, SEM, EDX, and XPS and compared with the HEA. Nanostructured materials based on HEOs with improved properties for visible light-activated photocatalysis (PC) could be used in the future for the degradation of a broad variety of volatile organic compounds (VOCs) in air.

Research project supported by program „Excellence initiative – research university” for the AGH University of Krakow, Grant No. 9705.

#### **Biography:**

Assistant professor at the Faculty of Non-Ferrous Metals at the AGH University Krakow. Author of more than 30 publications in the field of electrochemistry and materials engineering. Has knowledge in the field of synthesis of materials with electrocatalytic properties and materials with modified surface morphology for applications in hydrogen evolution.

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## Oral Talk

### Characterization of lipidic nanoformulations encapsulating the antifungal drug natamycin

*Luigi Talarico 1,2,3 , Ilaria Clemente 1,3 , Alessandro Gennari 1 , Giulia Gabbricci 1,3 ,  
Simone Pepi 1,2,3 , Gemma Leone 1,2,3 , Claudia Bonechi 1,3 , Claudio Rossi 1,3 , Simone  
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*2 National Interuniversity Consortium of Material Science and Technology (INSTM), Siena  
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*3 Center for Colloids and Surface Science (CSGI), Siena Research Group, Via della  
Laustruccia 3, 50019 Sesto Fiorentino, Italy*

*4 Dompé Farmaceutici S.p.A, Via Campo di Pile SNC, 67100 L'Aquila, Italy;*

#### Abstract:

Infectious diseases play a major role among the causes of blindness worldwide. Due to its anatomy and direct exposure to the environment, the human eye is particularly vulnerable to fungal and parasitic infections, caused, e.g., by trauma from penetrating objects, carriage of microorganisms from adjacent structures, and use of contact lenses. Negligence in timely treatment often results in vision impairment. Fungal keratitis is a major cause of blindness in corneal diseases, and its topical treatment requires several eye-drop applications and may require additional injections or surgery. Natamycin, a tetraene polyene that acts by binding to the main component of fungal walls, ergosterol, thus blocking fungal growth, is one of the proposed antifungal drugs for topical treatments [1]. However, its low retention at the ocular surface and scarce penetration across inner ocular tissues pose significant challenges that could be overcome with the use of lipid nanovectors [2]. In this work, various lipid nanoparticles (LNP) Systems loaded with Natamycin are physicochemically characterized and compared in terms of dimensions and stability, studied by Dynamic Light Scattering, and morphology investigated by Small Angle X-ray Scattering and monodimensional and bidimensional Nuclear Magnetic Resonance, and encapsulation efficiency assessed with HPLC-DAD. Transethosomes and lipid nanoparticles were prepared and characterized, and their suitability as carriers for the antifungal drug natamycin was preliminarily evaluated. Characterizations evidenced that both types of lipid nanosystems possessed interesting properties as vectors for eye treatment via topical administration. Indeed, TEs and LNPs showed appropriate dimensions (100–200 nm), monodispersity, and stability in suspension as a result of their high zeta potential values and appropriate charges to facilitate the interaction either with the anterior or posterior ocular segments. SAXS/WAXS analysis revealed the different supramolecular structures of the two nanocarrier types and confirmed that the intercalation of natamycin in the bilayer can induce tighter packing and enhance structuring properties. <sup>1</sup>H NMR evidenced the presence of signals associated with both hydrophilic and

lipophilic moieties of natamycin in loaded transtethosomes and LNPs, showing that the antifungal was indeed intercalated in the bilayer; this was further confirmed by NOESY measurements.

#### References

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  - 2 Gorantla, S.; Rapalli, V.K.; Waghule, T.; Singh, P.P.; Dubey, S.K.; Saha, R.N.; Singhvi, G. RSC Adv. 2020, 10, 27835–27855
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## Oral Talk

### Tuning magnetism in graphene nanoribbons via strain and adatoms

*Pablo Moles\*<sup>1</sup>, Hernán Santos<sup>2</sup>, Francisco Domínguez-Adame<sup>1</sup> and Leonor Chico<sup>1</sup>*  
*<sup>1</sup>GISC, Departamento de Física de Materiales, Facultad de Ciencias Físicas, Universidad Complutense, Madrid, Spain*

*<sup>2</sup>Departamento de Física Aplicada, Facultad de Ciencias Ambientales y Bioquímica, Universidad de Castilla-La Mancha, Toledo, Spain*

#### Abstract:

The atomic precision achieved both in synthesis and in defect engineering in zigzag graphene nanoribbons (ZGNRs) opens new opportunities for detecting and manipulating magnetism at these systems, which is highly desirable for future applications. We propose a way to selectively enhance the magnetic response of ZGNRs by different means. Firstly, we analyze the role of induced strain as a way to tune their electronic properties. Using first principles and tight-binding (TB) methods, we consider uniaxial strain along the zigzag direction of a ZGNR, resulting in a smooth, albeit important, enhancement of its magnetic response. We attribute this increase to modifications in the band structure produced by the strain field. Furthermore, we also explore the tunability of the magnetic response via the presence of point defects, namely H atoms adsorbed in the ZNGR, focusing on the ferromagnetic edge configuration, which we find more adequate for such property tuning. We find that the magnetic moment varies with strain yielding robust discrete plateaus of integer magnetic moment in the defected ZGNRs. These plateaus can be explained by resorting to the band structure, being related to the half-metallic character of the gap opening with strain, which may be relevant for magnetic applications of graphene nanoribbons.

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- [3] González-Herrero, H. et al. Science 352.6284, 437-441 (2016)

**Biography:**

I obtained my bachelor's degree in Physics in 2021, followed by a Master's in Nanoscience and Advanced Materials at Universidad Complutense de Madrid. During my master's, I joined the GISC-UCM group, which focuses on the electronic properties of novel materials and nanostructures. I am currently pursuing a PhD with the group, conducting theoretical research on charge and spin transport in graphene nanostructures, particularly graphene nanoribbons and moiré systems. As part of this work, I have also collaborated with Dublin City University, Ireland, developing Green's function methods for transport in moiré systems.

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**Invited Talk****STEM characterization of III-V nanowires using 4D-STEM**

*Elisa García-Tabarés, Beatriz Galiana, Alicia Gonzalo, José Miguel Reynolds, Mario Santiuste*

*Universidad Carlos III de Madrid. Avda. Universidad 30, 28911 Leganés (Madrid), Spain*

**Abstract:**

In recent decades, the field of STEM/TEM characterization has undergone a significant transformation with the advent of advanced analytical techniques such as Differential Phase Contrast (DPC) and four-dimensional Scanning Transmission Electron Microscopy (4D-STEM). These methodologies have expanded the capabilities of electron microscopy beyond conventional imaging. DPC enables the measurement of differential phase shifts between orthogonally polarized electron beams transmitted through a specimen, making it a powerful tool for detecting local electric fields—an application of particular interest in semiconductor research [1]. On the other hand, 4D-STEM involves scanning a highly collimated electron beam across the sample while recording a diffraction pattern at each position. The resulting 4D dataset (2D real space + 2D reciprocal space) facilitates advanced analyses, including strain mapping and crystallographic orientation determination in nanostructures [2]. In this work, we present preliminary results obtained from III-V semiconductor nanowires to demonstrate the potential of these techniques. Figure 1 displays preliminary strain maps ( $\epsilon_{xx}$  and  $\epsilon_{yy}$ ) for the GaInP section, derived using open-source 4D-STEM analysis scripts [3]. The data indicate compressive strain in both x and y directions, with a more pronounced effect along the x-axis. These initial findings highlight the promise of 4D-STEM for nanostructure characterization. Further theoretical modelling is currently underway to enhance the interpretation and understanding of the observed phenomena.

Figure 1: Normal ( $\epsilon_{xx}$  and  $\epsilon_{yy}$ ) strain maps carried out on the GaInP region achieved by 4D-STEM

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[2] C. Ophus Microscopy and Microanalysis, 25 (3) 2019, DOI: 10.1017/S1431927619000497

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## Invited Talk

### **Microstructure and mechanical behavior of Zr-based ferritic ODS steels processed by different powder metallurgical routes**

*Teresa Leguey, Vanessa de Castro\*, Moisés Oñoro, María A. Auger University Carlos III de Madrid, Spain*

#### **Abstract:**

Oxide dispersion-strengthened (ODS) reduced-activation ferritic steels are considered one of the most promising materials for structural applications inside fusion reactor vessels, albeit their manufacturing processes and resulting properties still need to be optimized. In this work, the impact of different powder metallurgical routes on the final microstructure and mechanical behaviour of an ODS steel with nominal composition Fe14Cr-2W-0.3Zr-0.24Y (in wt %) has been investigated. Starting from pre-alloyed atomized powders, the precipitation of oxide nanoparticles in the steel matrix has been promoted via three different routes: controlled oxidation of the powder particles, conventional mechanical alloying, and controlled oxidation followed by mechanical alloying. All three materials were subsequently consolidated by hot isostatic pressing and underwent the same thermomechanical treatment (hot rolling) afterwards. Their microstructure has been characterized by scanning and transmission electron microscopy, with emphasis on the identification and analysis of secondary phases and nanoprecipitates present. Microhardness and tensile behaviour as a function of temperature have also been investigated. These results provide a detailed comparison of the effects of different oxidation and mechanical alloying routes on nanoprecipitate distribution and their influence on the resulting microstructure and mechanical properties.

#### **Biography:**

The Nanostructured and Multifunctional Materials group of the Physics Department (University Carlos III de Madrid) has extensive experience in the manufacturing and characterization of structural materials for fusion applications. The research team has a solid background in the mechanical and microstructural characterization of ODS RAFM steels at the nanoscale, as well as competence in designing and performing irradiation campaigns and a deep knowledge of several defect characterization techniques.

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## Oral Talk

### **Mechanical strain-induced degradation of magnetic properties in FeCo-2V alloy**

*Sirapob Toyting<sup>1\*</sup>, Christopher Harrison<sup>2</sup>, Stefan Michalik<sup>3</sup>, Alexis Lambourne<sup>4</sup>, Howard J. Stone<sup>1</sup>*

<sup>1</sup> *Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, UK*

<sup>2</sup> *School of Engineering, Cardiff University, Cardiff CF24 3AA, UK*

<sup>3</sup> *Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot OX11 0DE, UK*

<sup>4</sup> *Rolls-Royce Plc, PO Box 2000, Derbyshire, DE24 7XX, UK*

#### **Abstract:**

Iron-cobalt (FeCo) soft magnets possess the highest saturation magnetisation among soft magnetic materials, making them essential in various high-performance applications. However, their high cost limits their use to specialised sectors where performance demands justify the expense. Despite their advantages, the influence of mechanical operating conditions—particularly mechanical strain—on the magnetic properties of FeCo magnets remains insufficiently studied. Mechanical strain can degrade magnetic properties, potentially leading to device failure. This study investigates the effect of deformation on the magnetic properties of FeCo-2V alloy. A methodology combining mechanical testing, magnetic characterisation using a Single Sheet Tester (SST), Electron Backscatter Diffraction (EBSD) analysis via Kernel Average Misorientation (KAM) mapping, and loss separation analysis was employed. Samples were strained to different levels, and KAM mapping was conducted on undeformed, 1% strained, and 3.5% strained samples. Results showed that increasing strain elevated dislocation density, reflected in higher average misorientation angles. Magnetic properties were measured across five frequencies using SST. Hysteresis loops revealed that higher strain produced larger loop areas, with coercivity and core loss increasing with strain. Loss separation analysis focused on hysteresis loss, showing that samples with higher strain had larger hysteresis loss coefficients due to increased domain wall pinning by dislocations. This hindered domain wall motion, raising coercivity and core losses. These results demonstrate the significant impact of mechanical deformation on magnetic performance, underscoring the necessity to consider mechanical operating conditions when designing and applying FeCo-2V alloys for reliable performance.

## Biography:

I am currently pursuing a PhD in Materials Science and Metallurgy at the University of Cambridge, after completing my MPhil at Cambridge and a First-class BEng in Materials Science and Engineering at Imperial College London. My studies have been supported by the Royal Thai Government Scholarship and Rolls-Royce plc. My research focuses on aerospace and magnetic materials, and I have contributed to publications and internships in advanced fields like additive manufacturing.

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## Oral Talk

### **Extremely Low Resistivity Size Effect Enabled by Epitaxial Growth of Nickel-Cobalt Alloy Thin Films for Next-Generation Interconnects**

Ju Young Sung<sup>1\*</sup>, Chae Hyun Lee<sup>1</sup>, Ye Bin Lim<sup>1</sup>, In Su Oh<sup>1</sup>, Sang Hyeok Lee<sup>1</sup> and Sang Woon Lee<sup>1</sup>

*<sup>1</sup>Department of Energy System Research and Department of Physics, Ajou University, Gyenggi-do, 16499, Republic of Korea*

## Abstract:

As semiconductor interconnects are scaled below 10 nm, the resistivity of metal films increases by enhanced electron scattering; thus, suppressing the resistivity size effect is essential to prevent performance degradation in advanced semiconductor devices. Copper, despite its low bulk resistivity, exhibits a significant increase in resistivity at reduced thickness owing to its long electron mean free path (EMFP) of 39 nm. To overcome this limitation, we demonstrate the epitaxial growth of hexagonal close-packed (HCP) nickel-cobalt (NiCo) alloy thin films having a short EMFP of approximately 5 nm as an alternative interconnect material that significantly suppresses resistivity scaling.

Density Functional Theory (DFT) calculations show a short EMFP of 5 nm for HCP NiCo alloy. However, NiCo alloys with 50–80 at% Co typically exhibit a mixture of HCP and face-centered cubic (FCC) phases, hindering single-phase HCP formation. To date, single-phase HCP NiCo films have not been experimentally realized. In this work, we introduce an HCP cobalt seed layer enabling, for the first time, the epitaxial growth of single-phase HCP NiCo films by minimizing lattice mismatch with the sapphire substrate.

This approach resulted in single-phase HCP NiCo films with an extremely low resistivity size effect. The films exhibited a resistivity of 19.83  $\mu\Omega\cdot\text{cm}$  at a thickness of 4.9 nm, markedly lower than that of copper at similar dimensions. This improvement is attributed to the short EMFP ( $\sim 5$  nm) of the HCP NiCo phase, which reduces electron scattering. These findings highlight the potential of phase-controlled HCP NiCo films to overcome interconnect scaling limitations.

**Biography:**

Ju Young Sung is a Ph.D. candidate under the supervision of Prof. Sang Woon Lee at Ajou University. She received her bachelor's degree in Electrical and Computer Engineering from Ajou University. Her research focuses on advanced metal thin films for next-generation memory devices. She aims to optimize the structural, electrical, and interfacial properties of these materials to enhance device performance.

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**Oral Talk****Achievement of Single-Phase Body-Centered Cubic CoMo Alloy Thin Films with Reduced Resistivity Size Effect**

*Ye Bin Lim<sup>1\*</sup>, Ju Young Sung<sup>1</sup>, Chae Hyun Lee<sup>1</sup>, In Su Oh<sup>1</sup>, Sang Hyeok Lee<sup>1</sup>, and Sang Woon Lee<sup>1</sup>*

*Department of Physics/Department of Energy Systems Research, Ajou University, Republic of Korea*

**Abstract:**

Conventional copper (Cu) interconnects suffer from a rapid increase in resistivity at linewidths below 10 nm due to enhanced electron scattering at surfaces and grain boundaries, attributed to Cu's long electron mean free path (EMFP). To overcome this resistivity size effect, the development of alternative metals and alloys with EMFP shorter than 5 nm has emerged as a key challenge for next-generation semiconductor technologies.

In this study, we report the first experimental realization of single-phase body-centered cubic (BCC) CoMo alloy thin films fabricated by a co-sputtering process. The deposition was achieved for the first time with the aid of a Mo seed layer. The films exhibited uniform composition and smooth surfaces in the nanometer thickness range below 10 nm. The resistivity as a function of CoMo film thickness was analyzed using the Fuchs-Sondheimer (FS) and Mayadas-Shatzkes (MS) models to quantitatively evaluate electron scattering mechanisms. The EMFP of BCC CoMo alloy was predicted to be approximately 5 nm based on the density functional theory (DFT) calculations, implying a weak resistivity size effect due to its short EMFP. However, the measured resistivity was significantly higher than predicted, even though the desired BCCCoMo structure was achieved. This discrepancy is attributed to enhanced electron scattering caused by the mismatch in the density of states (DOS) band centers and atomic radii between Co and Mo. These findings highlight the limitations of conventional resistivity prediction approaches and underscore the need for advanced models that account for alloy-specific electronic and structural characteristics in nanoscale interconnect applications.

**Biography:**

Ye Bin Lim received a B.S. degree in Physics from Ajou University, South Korea, and is currently pursuing an M.S. degree in the same department. Her research centers on metallic

thin films for semiconductor applications, with a particular focus on deposition, structural analysis, and electron scattering mechanisms in alternative interconnect materials. She recently demonstrated the sputter-based fabrication of single-phase BCC CoMo alloy thin films and investigated their resistivity size effect, emphasizing the role of structural and electronic factors in intermetallic systems.

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## Oral Talk

### **Porous silicon structural, morphological and optical properties enhancement after doping with Nd<sub>2</sub>O<sub>3</sub>**

*Ismail Selmi<sup>\*1</sup>, Imen Hammami<sup>1</sup>, and Beya Ouertani<sup>1,2</sup>*

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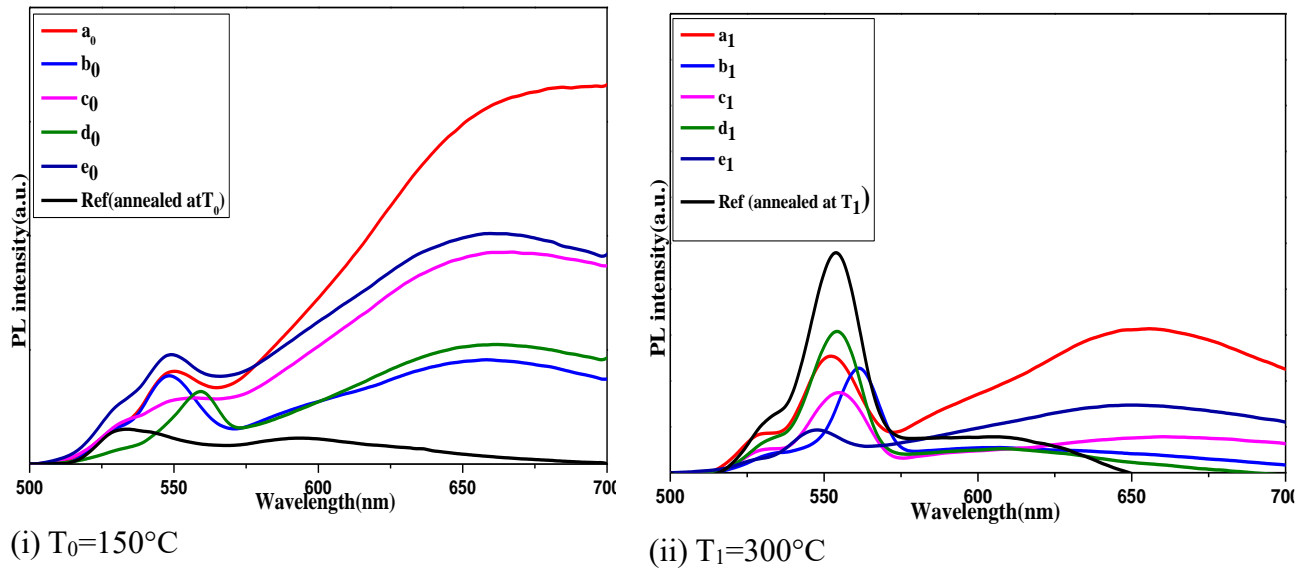
*<sup>2</sup>University of Carthage, Higher Institute of Environmental Science and Technology of Borj Cedria, Borj-Cedria Science and Technology Park, Tunisia*

#### **Abstract:**

The present work is interested in the enhancement of the optical properties of PSi to better pave the way for its integration in photovoltaic applications, its rare earth (RE) doping leads to obtain Nd<sub>2</sub>O<sub>3</sub>/PSi structure making it a promising material thanks to its anti-reflective and light trapping properties. Hence, in a first step, PSi samples were fabricated by electrochemical anodization technique of p type crystalline silicon (c-Si(100)) wafers in HF/EtOH solution with current density of 10mA/cm<sup>2</sup> and for 10min. In a second step, neodymium oxide (Nd<sub>2</sub>O<sub>3</sub>) with various molar concentrations (0.01, 0.02, 0.03, 0.04, and 0.05M) was deposited on the pre-prepared PSi substrates by the simple and low cost chemical deposition method. The as obtained samples, were immediately annealed at different heat temperatures (T<sub>0</sub>=150, T<sub>1</sub>=300, T<sub>2</sub>=400, T<sub>3</sub>=500, and T<sub>4</sub>=600°C). The structural, morphological and optical properties of the prepared Nd<sub>2</sub>O<sub>3</sub>/PSi structures were investigated by studying minority carrier lifetime ( $\tau_{\text{eff}}$ ) measurements, X-ray diffraction (XRD), Fourier transmission infrared spectroscopy (FTIR), spectroscopy energy dispersive X-ray (EDX), scanning electron microscopy (SEM), photoluminescence spectroscopy (PL) and reflectivity measurements.  $\tau_{\text{eff}}$  was enhanced for all the Nd<sub>2</sub>O<sub>3</sub>/PSi structures and, particularly, from 7.84  $\mu$ s for the untreated PSi (reference) to around 22.97 and 33.34  $\mu$ s for certain treatment conditions. The XRD patterns confirm the formation of a cubic crystal phase (c- Nd<sub>2</sub>O<sub>3</sub>) for the samples treated at T<sub>0</sub>=150, T<sub>2</sub>=400 and T<sub>4</sub>=600°C, while a hexagonal crystal phase (h- Nd<sub>2</sub>O<sub>3</sub>) was detected at T<sub>1</sub>=300 and T<sub>3</sub>=500°C heat treating. The FTIR spectroscopy study supports the XRD analyses which confirm the incorporation of Nd particles in the PSi structure. Moreover, it was detected the appearance of new Nd-O-Si vibration bonds peaked at around  $\sim 749$  cm<sup>-1</sup>, and Nd-O bonds replacing the unstable Si-H bonds. EDX analyses prove

the presence of Si, O, and Nd, in the prepared structures. The PL measurements showed two PL bands, in the blue-green and yellow-red ranges. Furthermore, the incorporation of Nd into the PSi structure leads to a remarkable decrease of the reflectivity from 18% for the annealed PSi (reference) to around 4% and 8%. These obtained interesting results confirm the wise choice of the Neodymium as dopant of the PSi for enhancing its efficiency acting as antireflection and passivation.

**Keywords:** PSi, Rare earth oxide,  $\text{Nd}_2\text{O}_3$ , Nd-O bonds, Nd-O-Si bonds, chemical deposition method, PL, Reflectivity, EDX, SEM,  $\tau_{\text{eff}}$ , FTIR, and XRD.



**Figure.12:** PL spectra of Nd-doped PSi with the different concentrations (a, b, c, d, e) after heat treatment at different temperatures ( $T_0=150$ , and  $T_1=300^\circ\text{C}$ ) for 30min in an infrared furnace in air atmosphere, The PSi (Ref) was annealed at the same temperature as the Nd-doped PSi .

#### Biography:

Ismail Selmi obtained his Baccalaureate diploma in Mathematics at El Ala high school, his bachelor's degree in physics, and his master's degree in Materials and nanostructures at the University of Science of Monastir-Tunisia. During the last three years, he has been a PsthD student at the Faculty of Science of Tunis at the University of Tunis El Manar, and he is a researcher at the Photovoltaic Laboratory (LPV) at the Research and Technology Center of Energy (CRTE), Science and Technology Park of Borj Cedria-Tunisia. He is working on silicon and porous silicon and their doping in the aim to improve their properties for solar cell applications.

## Invited Talk

### Innovative Bio-Composites for Noise Reduction

Dehenenet Flatie Tassaw<sup>1,2\*</sup>, Marcin Barbruski<sup>1</sup>, Adam Plich<sup>3</sup>, Tsegaye Lemmi<sup>1</sup>

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*<sup>2</sup>Textile Faculty, Ethiopian Institute of Textile and Fashion Technology, Bahir Dar University,  
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*\* Corresponding author*

#### Abstract:

Noise pollution, now the second leading environmental health threat in Europe after air pollution, affects over 20% of the EU-27 population due to increasing urbanization and industrialization. This study focuses on developing a sustainable, lightweight, and flexible acoustic bio composite panel using natural cellulosic fibers (sisal, flax, hemp), hollow glass microspheres (HGM), and a bio-based polyurethane (PU) matrix. The composites aim to enhance sound absorption, mechanical strength, and thermal stability. Fabrication was done through both one-shot and in-situ polymerization, with fibers added at 5–15% and HGM at 2–6% by weight of PU. Preliminary experiments used a controlled molding process for uniform dispersion. Acoustic insulation properties were assessed using an impedance tube (0–1600 Hz). A reference PU-HGM composite without fiber showed a low absorption coefficient of 0.14 at 500 Hz. Adding sisal fiber improved this to 0.18 due to its porous structure. Further enhancement was observed by integrating a woven natural fabric layer, increasing the coefficient to 0.30, highlighting the benefits of surface texturing and multilayer damping. All samples demonstrated strong absorption above 1000 Hz (coefficient >0.7), due to enhanced sound interaction with fiber-microsphere networks. These bio-composites show promising potential as eco-friendly acoustic materials for green buildings, automotive interiors, and industrial noise control systems.

**Key words:** Bio-based polyurethane, Hollow glass microsphere, Natural Fiber, Fiber reinforced composite, Acoustic, Sound absorbency.

#### Biography:

**Dehenenet Flatie Tassaw** is a PhD candidate in Materials Engineering at Lodz University of Technology, Poland. specializing in bio-composites development. He is also a lecturer and researcher at the Ethiopian Institute of Textile and Fashion Technology, Bahir Dar University. His research focuses on biomaterials, biopolymers, fiber-reinforced composites, material characterization, sustainable materials, process optimization, and nanomaterials. He holds an MSc in Fiber Science and Technology and has published several research articles related to fiber science, biomaterials, nanomaterials, and advanced textile applications. His academic work contributes to the development of sustainable and high-performance materials for environmental, industrial, and life science applications.

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## Day 2, Room B

### Invited Talk

#### **Infrared nanosecond pulse laser polishing improves the corrosion behaviour in simulated body fluid (SBF) of Ti6Al4V fabricated by electron beam powder bed fusion (EB-PBF) and laser beam powder bed fusion (LB-PBF)**

Juan Ignacio Ahuir-Torres<sup>1,\*</sup>, Guilherme Arthur Longhitano<sup>2</sup>, Onur Yuksel<sup>1</sup>, Viknash Shagar<sup>1</sup>, David Hitchmough<sup>1</sup>, Musa Bashir<sup>3</sup>, Hiren Kotadia<sup>1</sup>, Rob Darlington, and Eduardo Blanco-Davis<sup>1</sup>

<sup>1</sup>*School of Engineering, Liverpool John Moores University, Liverpool L3 3AF, UK*

<sup>2</sup>*Faculdade de Engenharia Mecânica, Universidade Estadual de Campinas (UNICAMP), 13083-860, São Paulo, Brazil.*

<sup>3</sup>*Civil and Environmental Engineering, University of Liverpool, Liverpool, L69 7ZX, UK*

#### **Abstract:**

Additive manufacturing is a powerful technology that enables the design of Ti6Al4V (titanium alloy) structures with complex shapes that are highly relevant in the biomedical industry to create implants. Among additive manufacturing techniques, electron beam powder bed fusion (EB-PBF) and laser beam powder bed fusion (LB-PBF) stand out in manufacturing metallic implants with complex morphologies. However, the lateral surface of the samples generated using both methods often exhibits numerous imperfections such as cracks, high roughness, voids, and non-melted residue powders. These imperfections reduce the corrosion resistance of the manufactured materials in biofluids, thereby diminishing the service life of implants. Laser polishing can potentially remove these imperfections, enhancing the additive-manufactured implants' corrosion resistance. Nonetheless, traditional continuous wave laser polishing alters the microstructure of the additively manufactured samples, potentially degrading their properties. The nanosecond laser polishing can avoid this handicap. The present work studies surface polishing using an infrared nanosecond pulsed laser on EB-PBF and LB-PBF manufactured samples. The corrosion resistance of the laser-polished and non-polished samples was evaluated in a simulated body fluid using various electrochemical analysis techniques, including electrochemical noise, potentiodynamic polarisation curve, and electrochemical impedance spectroscopy. The laser processing effectively decreased the roughness of the samples, which improved the breaking passive film potential and reduced the chemical activity of the passive film. The samples manufactured by EB-PBF exhibited the highest passive film break potential. These findings highlight the potential of nanosecond laser processing to enhance the longevity of additively manufactured titanium implants.

**Biography:**

Juan Ignacio Ahuir-Torres is currently a Research Fellow at Liverpool John Moores University. He received his physical chemistry PhD with specialisation in electrochemistry from the Universidad Autónoma de Madrid. He has contributed to multiple funded research projects, including EPSRC, InnovateUK, Horizon 2020 and Horizon Europe. His scholarly works have been published in several high-impact journals, including *Electrochimica Acta*, *Material Degradation* and *Material Today Communications*. He has also presented his research investigations at internationally recognised congresses and symposiums, including EUROMAT and CNTMAT. His research fields encompass biomaterials, laser processing, corrosion, electrochemistry, molecular dynamics, and tribology.

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**Invited Talk****Characterization of Pharmaceutical Tablets under Diametral Compression using DIC and SEM**

Alex Fok<sup>1\*</sup>, Sara Ong<sup>1</sup>, Zijian Wang<sup>2</sup> and Calvin Sun<sup>2</sup>

*<sup>1</sup>Minnesota Dental Research Center for Biomaterials and Biomechanics, School of Dentistry, University of Minnesota, USA; <sup>2</sup>Department of Pharmaceutics, College of Pharmacy, University of Minnesota, USA*

**Abstract:**

Mechanical properties such as Young's modulus, Poisson's ratio and fracture strength are important parameters for pharmaceutical tablets during their manufacture and packaging. While the disc in diametral compression is routinely used to measure the fracture strength of tablets, it is currently not used to measure other mechanical properties. Here, we propose using digital image correlation (DIC) to measure the full-field surface strains of tablets under diametral compression. Together with stresses given by the Hertz analytical solution, Young's modulus and Poisson's ratio of the tablet can be estimated in addition to its fracture strength. This method can thus reduce or even eliminate the need for other tests to measure the elastic properties, reducing the costs involved in quality control and product development.

To verify the proposed method, microcrystalline cellulose (MCC) tablets fabricated with different compaction pressures were tested under diametral compression while their surface strains were being captured by DIC. Isotropic, generalized Hooke's law with the plane-stress condition was assumed for the material on the tablet surface, with the two equations relating the direct stresses and strains used to derive its Young's modulus and Poisson's ratio. The values of these properties as a function of porosity agreed well with published data.



Furthermore, the full-field strain measurements allowed assessment of the heterogeneity of the tablets and the stress-dependence of Young's modulus, which had a lower value in tension than in compression. The latter behavior was attributed to the crack-like defects, revealed with SEM, that can only be opened up by tension.

### **Biography:**

Professor Alex Fok is the current director of the Minnesota Dental Research Center for Biomaterials and Biomechanics (MDRCBB). The MDRCBB is an international leader in the development and application of novel characterization techniques for dental biomaterials, with long-standing collaboration with dental materials manufacturers. Professor Fok's research focuses on the material characterization, nondestructive examination, lifetime prediction and shape optimization of dental restorations. A principal aim of his research is to instill more engineering principles and analytical techniques into the design and assessment of dental restorations and treatments so as to improve their longevity and effectiveness.

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## **Invited Talk**

### **Nano-Topographic Cues: the Role in T Cell Stimulation and Immunotherapeutic Applications**

*Mark Schwartzman*

*Department of Materials Engineering, (2) Ilse Katz Institute for Nanoscale Science and Technology, Ben-Gurion University of the Negev, Beer-Sheva, Israel*

### **Abstract:**

T cells, essential players in adaptive immunity, are activated through interactions between T-cell receptors and ligands on antigen-presenting or target cells. Recent evidence shows that physical factors—such as mechanical stiffness, nanoscale topography, and ligand clustering at the cell interface—significantly influence T-cell activation, though the underlying mechanisms remain unclear. Reductionist systems mimicking in vivo cues offer a promising strategy for investigation.

This talk will present recent advances in engineering nanoscale systems to study T-cell activation. First, we developed nanostructured platforms to explore how segregation of activating and inhibitory receptors impacts signaling. These systems use patterned nanodomains fabricated through high-throughput nanosphere lithography, angled evaporation, and orthogonal biofunctionalization. We also studied the effect of ligand clustering, finding that overall ligand density governs activation but can be compensated by nanoscale clustering.

In the second part, I will discuss mechanostimulatory platforms for generating immunotherapeutic T cells. We demonstrated that biomimetic surfaces with controlled elasticity and nanotopography optimize activation, reduce exhaustion, and enhance proliferation, differentiation, and CAR transfection. By fine-tuning these surfaces, we produced CAR T cells with superior cancer-killing potency compared to standard methods. Finally, I will highlight a novel dry-assembly colloidal lithography approach enabling scalable fabrication of these biomimetic surfaces, now being integrated into commercial bioreactors for large-scale CAR T cell production.

### **Biography:**

Mark Schwartzman is a Professor of Materials Engineering at Ben-Gurion University, specializing in the physical interactions between immune or cancer cells and their microenvironment. He earned his B.Sc. and M.Sc. from Technion, Ph.D. from Columbia University, and completed postdoctoral training at the Weizmann Institute. His main research areas include: (1) investigating how spatial ligand organization regulates T cell and NK cell activation using nanofabricated platforms; (2) exploring mechanical contact guidance—cell migration driven by stiffness patterning—using engineered micropatterns; and (3) designing topographic, elastic surfaces to improve CAR T cell activation and expansion, validated through in vitro and in vivo studies.

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## **Invited Talk**

### **Surface Modification of Cellulose with Amino Groups for Antibacterial Functionality**

Paola Costanzo<sup>1\*</sup>, Federica Meringolo<sup>1</sup>, Ester Rosa<sup>2</sup>, Giorgia Puleo<sup>3</sup>, Loredana Maiuolo<sup>1</sup>, Vincenzo Algieri<sup>4</sup>, Antonio Jiritano<sup>1</sup>, Antonio De Nino<sup>1</sup>, Floriana Campanile<sup>2</sup> Giuseppe Arrabito<sup>3</sup>.

<sup>1</sup>*Department of Chemistry and Chemical Technologies, University of Calabria, Italy;*

<sup>2</sup>*Department of Biomedical and Biotechnological Sciences, University of Catania, Italy;* <sup>3</sup>

*Department of Physics and Chemistry-Emilio Segrè, University of Palermo, Italy;* <sup>4</sup> *IRCCS NEUROMED—Mediterranean Neurological Institute, Italy.*

### **Abstract:**

Cellulose is a comparatively low-cost, bio-based, and renewable material with various profitable properties, like non-toxicity, biocompatibility, and biodegradability. Its chemical-physical characteristics make it particularly suitable for the development of materials with advanced technological properties, especially in the biomedical field. In the present work, metal-cellulose composites were designed and prepared for the production of new non-drug antimicrobial agents, which represents a global challenge due to the microbial resistance to

antibiotics (AMR), resulting from their worldwide misuse. Both cellulosic papers and powders were functionalized with various amino groups, achieving a good grafting percentage and emulating the inherent bactericidal properties of chitosan. These materials, also obtained from renewable resources derived from agri-food wastes, were chemically modified through the alkoxysilane technique in non-toxic solvents. The obtained amino-cellulosic materials were characterized by SEM-EDX, FTIR spectroscopy, and tested as carriers for ZnO nanoparticles. ZnO in the form of nanostructured material has shown potential for photocatalytic and antibacterial applications, due to the release of reactive oxygen species and zinc ions. These composites provide stable platforms for ZnO's prolonged release biomedical applications, with preliminary results confirming antibacterial efficacy against Gram-positive and Gram-negative bacteria.

The Italian Ministry of University and Research is acknowledged for funding through the PRIN 2022 project "SOTERIA" PNRR M4.C2.1.1. 2022WZK874 - CUP: H53D23004700006

### **Biography:**

Prof. Paola Costanzo is an associate professor in Organic Chemistry. She is the co-author of over 50 papers in peer-reviewed international journals. In 2020, she received the Junior Research Award for Organic Chemistry in its Methodological Aspects for her studies focused on the realization of eco-sustainable methodologies by using unconventional reactors for the development of alternative and effective ways for synthetic processes in the chemical and pharmaceutical industries. Her research interests focus on the green synthesis of heterocycles with potential biological activity and on chemical modifications of biomaterials to obtain new advanced tools for water remediation and biotechnological applications.

## **Oral Talk**

### **Electrospinning Multi-Polymer Nanofibers Based on Gelatin, Sodium Alginate, PVA, and Pectin for Biomedical Applications**

*Huynh-Ngoc-Truc Nguyen<sup>1</sup>\*, and Chuan-Li*

*<sup>1</sup>Department of Biomedical Engineering, National Yang Ming Chiao Tung University, Taipei City, Taiwan 11221*

### **Abstract:**

Composite nanofibers exhibiting improved mechanical strength, biological compatibility, and regulated degradability are essential for numerous biomedical applications, such as tissue engineering, wound healing, and targeted drug administration. Among various fabrication methods, electrospinning has emerged as a highly versatile and efficient technique to generate nanofibrous scaffolds that structurally and functionally resemble the native extracellular

matrix. Nevertheless, engineering nanofibers that integrate multiple functionalities in a single, biocompatible platform remains a significant challenge. In this study, we developed electrospinning nanofibers composed of gelatin, sodium alginate (SA), polyvinyl alcohol (PVA), and pectin - a novel four-component polymeric system designed to combine structural integrity, bioactivity, and biodegradability synergistically. The optimized formulation at a volumetric ratio of Gelatin:SA:PVA:Pectin (30:10:40:20 v.%) produced bead-free fibers with uniform morphology and an average diameter of  $233.32 \pm 27.7$  nm, confirmed via scanning electron microscopy (SEM). Fourier-transform infrared (FTIR) spectroscopy demonstrated enhanced hydrogen bonding, intermolecular interactions, and overall scaffold stability. Rheological assessments indicated advantageous viscosity and surface tension, guaranteeing consistent fiber production. Biological evaluations utilizing HeLa cells demonstrated elevated cytocompatibility, exceeding 85% viability, with robust cellular adhesion and proliferation. The nanofibers enabled the prolonged release of embedded bioactive chemicals, highlighting their effectiveness in regulated drug delivery systems. This multi-polymer technique offers a more comprehensive answer for biological material design than typical binary systems. Current efforts focus on incorporating stimulus-responsive behavior and evaluating scalability for clinical use.

### **Biography:**

Huynh-Ngoc-Truc Nguyen, born on April 18, 1997, received her M.S. degree in 2023 from the Graduate Institute of Biomedical Materials and Tissue Engineering, College of Biomedical Engineering, Taipei Medical University, Taipei, Taiwan. She is currently pursuing a Ph.D. in Biomedical Engineering at the College of Biomedical Science and Engineering, National Yang Ming Chiao Tung University, Taipei, Taiwan. Her research focuses on the development and application of nanoparticles, biomedical materials, hydrogels, and electrospinning nanofiber technologies for advanced therapeutic and tissue engineering applications.

## **Oral Talk**

### **Cell/derived ECM loaded PCL/Chitosan nanofibers for improved periodontal tissue regeneration strategies**

#### **Abstract:**

The periodontium is a hierarchical structure composed of specialized tissues promoting tooth support and stability. Bacterial dental plaque accumulation causes periodontitis, a chronic inflammatory infection of the periodontium, that, if not treated, can lead to tooth loss. Current regenerative treatments fail to effectively promote a complete and coordinated periodontal regeneration, hence the a demand for alternative strategies to improve clinical outcomes. Decellularized ECM (dECM) has been explored for tissue engineering applications since it can mimic the in vivo microenvironment, offering the opportunity to enhance the bioactivity of the scaffolds.

In this work, electrospun polycaprolactone/chitosan (PCL/CTS) nanofibrous scaffolds loaded with cell-derived extracellular matrix (ECM) were developed using lyophilized dECM derived from human Periodontal Ligament Stem Cells (hPDLSCs).

Characterization of hPDLSCs and dECM was performed with regard to morphology, protein expression, and DNA, glycosaminoglycans, and collagen contents. hPDLSCs were differentiated into the osteogenic lineage on PCL, PCL-CTS, and PCL-CTS-ECM scaffolds for 21 days.

After decellularization, dECM maintained the expression of proteins, displayed a fibrillary structure, and retained glycosaminoglycan and collagen contents. The obtained results demonstrate that PCL-CTS-ECM scaffolds significantly promoted cell proliferation in comparison to PCL and PCL-CTS scaffolds, due to the presence of dECM. PCL-CTS-ECM scaffolds enhanced the osteogenic differentiation of hPDLSCs, confirmed by increased alkaline phosphatase (ALP) activity and calcium deposition. PCL-CTS-ECM scaffolds exhibited a statistically significant increase in ALP and Collagen I gene expression.

Overall, our results show that dECM-loaded electrospun scaffolds enhanced the proliferation and osteogenic differentiation of hPDLSCs. To our knowledge, this work describes the first use of lyophilized cell-derived ECM in combination with electrospun nanofibrous scaffolds for periodontal tissue engineering applications, highlighting its potential as a promising alternative treatment strategy for periodontitis.

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## Invited Talk

### **H<sub>2</sub>O and CO<sub>2</sub> interaction with perovskitic (110) surface: the case of SrFeO<sub>3</sub>**

*Mario Italo Trioni<sup>1\*</sup>, Fausto Cargnoni<sup>1</sup>, Massimo Viviani<sup>2</sup>, Livia Giordano<sup>3</sup>*

*<sup>1</sup>National Research Center of Italy (CNR), SCITEC, Milano, Italy*

*<sup>2</sup>National Research Center of Italy (CNR), ICMATE, Genova, Italy*

*<sup>3</sup>University of "Milano-Bicocca", Dept. of Material Science, Milano, Italy*

#### **Abstract:**

The transition to renewable energy sources is one of EU flagship projects. Reaching the CO<sub>2</sub> reduction target set by EU (climate-neutrality by 2050), requires the development of energy storage or conversion technologies to be coupled with intermittent renewable energy sources. Solid oxide electrolysis cells (SOECs) present several advantages in this context.

Simultaneous CO<sub>2</sub> and water electrolysis in one device has the advantage of consuming CO<sub>2</sub> and producing syngas (H<sub>2</sub> + CO). Despite its appeal, CO<sub>2</sub>/steam co-electrolysis is currently limited by stability and electrochemical activity issues of state-of-art materials.

Understanding the reaction mechanisms and improving the reaction kinetics at the solid-gas interfaces on electrodes of SOECs have the potential to lower operational temperatures, thus hindering parasitic reactions that limit their stability and lifecycle, and expanding the range of materials that can be used in these cells. In general, reaction kinetics are influenced by

thermodynamic quantities such as gas partial pressure and temperature, but they also strongly depend on the nature and availability of active sites. Electrode reactions further require charge transfer between adsorbed species and the solid electrode, meaning that the applied electric potential is another factor influencing overall kinetics. A detailed understanding of the oxide structure—especially of point defects, which may act as active sites at the solid-gas interface—and the adsorption energetics of reaction intermediates are essential for modeling electrode reactions and optimizing materials. This work presents first-principles results on the interaction of H<sub>2</sub>O and CO<sub>2</sub> with the SrFeO<sub>3</sub>(110) surface, which take into account all these aspects.

### Biography:

**Mario Italo Trioni**, researcher at CNR-SCITEC, bachelor's degree and Ph.D. in Physics at the “Università degli Studi” of Milano. His main research interests are related to theoretical ab-initio study of solid surfaces and molecule-surface interaction with focus on the magnetic, electronic, and electron transport properties. He is author of more than hundred publications. Other topics of interest are low dimensional carbon systems (graphene, nanoribbon and nanoflakes) and defective oxide surfaces.

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### Invited Talk

#### Composition, structure and phonon softening in high entropy alloys based on PbTe thermoelectrics

*NM Nemes<sup>1\*</sup>, JM Gallardo-Amores<sup>1</sup>, N Biskup<sup>1</sup>, JI Beltran<sup>1</sup>, F Serrano-Sánchez<sup>2</sup>, H Lyder Andersen<sup>2</sup>, JA Alonso<sup>2</sup>, JL Martínez Peña<sup>2</sup>, OJ Durá<sup>3</sup>, MT Fernández-Díaz<sup>4</sup>, J. Gainza<sup>5</sup>*

*<sup>1</sup>Universidad Complutense de Madrid, Spain*

*<sup>2</sup>Instituto de Ciencia de Materiales de Madrid, Spain*

*<sup>3</sup>Universidad de Castilla-La Mancha, Ciudad Real, Spain*

*<sup>4</sup>Institut Laue-Langevin, Grenoble Cedex, France*

*<sup>5</sup>European Synchrotron Radiation Facility, Grenoble Cedex 9, France*

### Abstract:

We stabilized high-entropy alloys (HEAs) using high-pressure synthesis of the excellent thermoelectrics PbTe and SnSe, incorporating over 10% Sn, Se, and Sb simultaneously. However, Ge is consistently rejected by the PbTe/GeTe structure. HEAs typically form cubic or hexagonal structures with large unit cells of at least four atoms, none being minority dopants. They hold promise in many fields, especially thermoelectrics [1].

Few HEAs have been successfully stabilized, particularly intermetallic ones, making our PbTe-based HEAs significant. Their simple crystallography but complex stoichiometry makes determining the actual stabilized phase difficult, requiring neutron and x-ray

diffraction. Studying disorder evolution upon alloying provides insights into phonon lifetime changes. Anharmonic responses to external parameters like temperature and pressure can renormalize phonon frequencies and/or enhance atomic displacement parameters (ADPs) beyond quasi-harmonic expectations.

A thorough analysis of low-temperature ADPs ( $U_{\text{iso}}$ ) reveals large static distortions, indicating expected compositional disorder. Temperature-dependent ADP analysis using the Einstein model, compared with phonon density of states from INS, gives insights into local structure and HEA formation. Comparing with inelastic neutron spectroscopy and ab-initio calculations is crucial, as shown for SnSe alloyed with Ge or Sb [2-4].

We studied HEAs of nominal compositions  $\text{Pb}_{2.5}\text{SnTe}_3\text{Se}$ ,  $\text{Pb}_{2.5}\text{SnSbTe}_3$ , and  $\text{Pb}_{2.5}\text{SnSbTe}_3\text{Se}$ , comparing them with PbTe.

We thank the ILL, ESRF, and ALBA for facilities. Electron microscopy observations were carried out at the Centro Nacional de Microscopia Electronica (CNME-UCM). Funding was provided by MCIN/AEI (grant nos. PID2021-122477OB-I00, TED2021-129254B-C21, TED2021-129254B-C22, RYC2021-033518-I) and NextGenerationEU.

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## Biography:

Norbert M. Nemes, an experimental solid-state physicist, earned his PhD from the University of Pennsylvania in 2002. After postdoctoral work at NCNR-NIST and the Materials Science Institute of Madrid, he became a Full Professor at Universidad Complutense de Madrid, where he directs the Magnetometry and High-Pressure Synthesis labs. He has published over 150 papers (h-index 30) on low-dimensional materials, superconductors, spintronics, magnetic anisotropy, and multifunctional materials. In recent years, his research has focused on thermoelectrics.

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## Invited Talk

### Enhancing Supercapacitor Performance through Mn-Doped ZnO: A Defect Engineering Approach

*Ameen Uddin Ammar<sup>1\*</sup>, Arpad Mihai Rostas<sup>2</sup>, Dana Toloman<sup>3</sup>, Adriana Popa<sup>4</sup> and Maria Stefan<sup>5</sup>*

*National Institute for Research and Development of Isotopic and Molecular Technologies,  
Cluj-Napoca, Romania*

#### **Abstract:**

Inducing defects in metal oxide materials via doping with transition metal ions is a well-established strategy to enhance the electrochemical performance of supercapacitors. In this study, we synthesized manganese (Mn)-doped zinc oxide (ZnO) and evaluated its potential as an electrode material for supercapacitor applications. A comprehensive analysis of the defect environment in both undoped and Mn-doped ZnO was conducted using electron paramagnetic resonance (EPR) and photoluminescence (PL) spectroscopy. These techniques revealed the evolution of defect centers as a function of Mn doping concentration, offering insights into their role in electrochemical performance. Among the synthesized samples, ZnO doped with 0.6% Mn exhibited the highest specific capacitance of 163 F/g at a scan rate of 10 mV/s, along with excellent cyclic stability, retaining 95% of its initial capacitance after 500 cycles. This study highlights the significance of defect engineering in metal oxides for energy storage applications and underscores Mn-doped ZnO as a promising candidate for high-performance supercapacitors.

#### **Biography:**

Ameen Uddin Ammar has been a scientific researcher at the National Institute for Research and Development of Isotopic and Molecular Technologies since March 2024. His research involves testing innovative electrode materials for supercapacitor applications by working on the defect structure. Ameen has published numerous papers on supercapacitor applications.

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## Invited Talk

### **Stoichiometry engineering of sputtered Molybdenum Oxide thin films as Hole-Selective Contact for Silicon Solar Cells**

*Maria Miritello\**

*CNR-IMM, Via S. Sofia, 64, I-95123 Catania, Italy*

#### **Abstract:**

Among the most efficient silicon solar cells, heterojunction (HJ) architecture has reached efficiencies exceeding 27%. The main feature relies on the use of thin amorphous hydrogenated Si (a)Si:H interlayers for surface passivation and charge transport. To further overcome HJ efficiency, the implementation of molybdenum oxide (MoO<sub>x</sub>) represents a promising alternative to p-doped (a)Si:H as a dopant-free hole-transport layer. It could reduce parasitic optical absorption and capital-intensive deposition processes involving hazardous gases, paving the way for a more efficient and eco-friendly cell solution.

This presentation will explore stoichiometry engineering of MoO<sub>x</sub> ultra-thin films deposited by magnetron sputtering, as an industrially scalable and cost-effective method. Since oxygen vacancies play a crucial role in film optical transparency, charge transport, and carrier selectivity, oxide stoichiometry has been demonstrated to be finely tuned between stoichiometric (O/Mo=3.0) to sub-stoichiometric (O/Mo=2.6). Also, Mo<sup>5+</sup> concentration, strictly correlated to O vacancies, has been correlated to film transparency, band gap, and work function values as a function of film stoichiometry.

Moreover, the role of the Si/MoO<sub>x</sub> interface in MoO<sub>x</sub>-based HJ will also be discussed. Data will evidence remarkable stability of sputtered MoO<sub>x</sub> films independently of stoichiometry. Moreover, energy band alignments, estimated by Surface Photovoltage, will reveal the strong dependence on Si surface pre-treatments, besides film stoichiometry. Thus, the best conditions to maximize HJ efficiency will be shown by demonstrating sputtering as a viable route for developing dopant-free selective contacts for next-generation PV technologies.

The study was partially funded by Horizon Europe Energy Project FreeHydroCells and MUR-PNRR project SAMOTHRACE.

#### **Biography:**

**Maria Miritello** is a Senior Researcher at the National Research Council. She received her PhD degree (cum laude) in Materials Science in 2007. Her research activity is mainly focused on innovative materials for advanced devices in photovoltaics and environmental fields. In particular, she develops materials synthesis by physical vapor deposition methods to reach a fine control of properties of rare earth-based compounds, transparent conductive, and metal oxides. She was involved in the organization and an invited speaker at several international conferences. She is the author of 115 papers on ISI scientific journals, holding an h-index of 29 and about 2700 citations (Scopus, 2025).

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## Invited Talk

### 4-Nitrophenol Reduction and Antibacterial Activity using Green-Synthesized Ag–Cu Bimetallic Nanocatalysts Immobilized on Modified Kaolin

Stavros G. Pouloupoulos\* and Awal Adava Abdulsalam<sup>1</sup>, Madina Pirman<sup>1</sup>, Tri Thanh Pham<sup>1</sup>

<sup>1</sup>Nazarbayev University, Astana, 010000, Kazakhstan

#### Abstract:

Industrial effluents often contain both hazardous organics like 4-nitrophenol (4-NP) and microbial pathogens. There is a growing demand for multifunctional catalysts capable of detoxifying pollutants and offering antimicrobial properties through sustainable synthesis routes. In this study, a green synthesis and dual-functional application of Ag–Cu bimetallic nanocatalysts immobilized on functionalized kaolin was presented for the catalytic reduction of 4-NP to 4-aminophenol and antibacterial activity. Raw kaolin was acid-treated and grafted with amine (–NH<sub>2</sub>) groups, creating –NH<sub>2</sub> anchoring sites. Silver and copper precursors were varied at different ratios and co-reduced on the modified kaolin using tannic acid. Catalytic activity was quantified by pseudo-first-order kinetics for 4-NP reduction with NaBH<sub>4</sub>, while antibacterial efficacy was assessed against *E. coli* and *S. aureus*. Results reveal that Ag:Cu (3:1) composite achieved complete 4-NP reduction in 7 min ( $k_{app} \approx 0.59 \text{ min}^{-1}$ ) and retained >97 % activity over five reuse cycles. Ag–Cu bimetallic catalysts showed improved antibacterial activity against *E. coli* and *S. aureus* compared to monometallic Ag, confirming synergistic antibacterial action. The use of tannic acid enabled an environmentally benign synthesis of a highly effective and reusable catalyst for both pollutant conversion and bacterial inhibition. This study introduces a scalable, low-cost, green nanocatalyst system with dual environmental and public health benefits, addressing pressing water pollution and antimicrobial challenges.

#### Biography:

Dr. Stavros G. Pouloupoulos is a Full Professor and Chair of the Department of Chemical and Materials Engineering at Nazarbayev University (Astana, Kazakhstan), widely recognized as a leading institution in Central Asia for its academic rigor, research excellence, and international outlook. His research interests include Chemical Reaction Engineering, Environmental Engineering, and the interaction between the Environment and Development. He has authored approximately 100 research articles, which have received 3,786 citations, and holds an h-index of 30.

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## Invited Talk

### The optical properties of Mn based halide compound semiconductors

*Bingsuo Zou\**

*(School of Resources, Environment and Materials, Guangxi university, Nanning 530004, China )*

#### **Abstract:**

-- Diluted magnetic semiconductors (DMS) are composed of typical semiconductors ZnO, CdS and ZnSe with the doping transition metal (TM) ions, which can give efficient emission and ferromagnetism. Their excitation come from the spins of TM (for example Mn) ions with exciton, often can be called “excitonic magnetic polaron”, whose behaviors strongly depend on the size of doped semiconductors. Here we presented a series of Mn halide compound and/or Mn doped halides, in which strong photoluminescence can be identified and enhanced by the interactions between confined exciton in  $(\text{MnX})_n$  cluster and optical phonons in the lattice, whose excitation show clear character of magnetic polaron in magnetic semiconductors, which supplied new concepts for designing luminescence materials in the future.

#### **Biography:**

Zoubs obtained a Doctorate from Jilin University in 1991, Nankai University as postdoctoral, then joined the faculty at the Institute of Physics, CAS in 1994; visited NUS and Georgia Tech as a visiting scholar in 1996-1999. In 2000, he came back to CAS China as a hundred-talent research scientist in the Institute of Physics. In 2005, he moved to Huna University in the School of Physics and Microelectronics. In 2006, he was nominated and enrolled as a Changjiang Scholar of MOE. In 2009, he joined BIT as dean of the School of MSE. In 2018, he joined Guangxi University and was appointed as the dean of REM in 2020. He obtained the second Prize of the 2019 National Natural Science Award.

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## Invited Talk

### Cobalt Ferrite Nanochessboard

*A. Lisfi*

*Dept. of Physics, Morgan State University, Baltimore, MD 21251*

#### **Abstract:**

In this study, we report the discovery of cobalt ferrite nanochessboard with superior magnetic properties over the well-known  $\text{CoFe}_2\text{O}_4$  inverted bulk phase. The patterned structure was stabilized in thin films through an epitaxial growth of  $\text{CoFe}_2\text{O}_4$  on an MgO substrate. It consists of periodically arranged normal and inverted spinel phases in the form of a nanochessboard with an average unit size of 20 nm. The synthesized nanochessboard exhibits a giant magnetization ( $570 \text{ emu/cm}^3$ ), much higher than that yielded by the fully inverted phase of single crystal  $\text{CoFe}_2\text{O}_4$  ( $400 \text{ emu/cm}^3$ ). Beside its ultra-large magnetization, the ceramic array manifests a soft magnetic character with much lower anisotropy than the one of the naturally occurring bulk phase, making the discovered structure very attractive to applications such as sensing, actuating, and magnonic devices. In the presentation, we will discuss the magnetization and the anisotropy results of the nanochessboard based on the magnetic moments of  $\text{Fe}^{3+}$  and  $\text{Co}^{2+}$ , their repartition among tetrahedral and octahedral sites and the magnitude and the sign of the anisotropy of  $\text{Co}^{2+}$  in both tetrahedral and octahedral sites. The presentation will cover the details of the nanochessboard synthesis and characterization including film growth by pulsed laser deposition, structural analyses done by TEM and XRD, and magnetic measurements performed with VSM and torque magnetometry. The discovered nanochessboard opens new research directions for engineering new magnetic oxides with enhanced properties that can fulfil the requirements of modern technology.

#### **Biography:**

Dr. Lisfi is a full professor in the Physics department at Morgan State University. His research is primarily on magnetic materials, including bulk and low-dimensional structures. He has a well-established lab of magnetic characterization, imaging, and materials synthesis. Dr. Lisfi is the recipient of competitive research awards from different funding agencies such as the NSF and the Air Force. He is currently the director of the CREST Center for Advanced Magnets and Semiconductors, funded by NSF in 2023. For the past years, he has been serving as a panelist and Ad hoc reviewer with NSF, as well as a reviewer for different journals.

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## Invited Talk

### Synergistic strengthening-toughening design and multiscale construction mechanisms of carbon aerogels

*Fuhua Xue<sup>1</sup>\*, Yunxiang Chen<sup>1</sup>, Qingyu Peng<sup>1</sup>*

*<sup>1</sup> Harbin Institute of Technology, China*

#### **Abstract:**

Carbon aerogels, owing to their ultralow density, exceptional thermal stability, and electrical conductivity, are emerging as versatile platforms for advanced applications in energy conversion and storage, pollutant adsorption, tissue engineering scaffolds, and flexible sensing. However, a persistent trade-off between mechanical strength and toughness in current carbon aerogels has significantly limited their reliability under extreme service conditions. Existing systems can be broadly categorized into two types: (1) networks assembled from low-dimensional nanomaterials such as carbon nanotubes (CNTs) or graphene, which exhibit outstanding toughness (elastic strain > 90%) but suffer from low compressive strength (< 200 kPa) due to weak interfacial interactions; and (2) resin-derived aerogels with highly crosslinked, brittle carbon skeletons that provide high strength (> 10 MPa) but minimal toughness (elastic strain < 3%), leading to catastrophic failure under load. In this study, we address this structural–mechanical bottleneck by employing CNTs as the primary building blocks and systematically tuning their nanoscale parameters—including diameter, junction morphology, and spatial distribution—to achieve synergistic enhancement of mechanical properties. As a result, we developed a novel CNT-based carbon aerogel that combines high compressive strength (up to 40 MPa) with improved toughness (elastic strain > 10%). Experimentally, we overcame the diameter constraints of conventional CVD-grown CNTs, achieving a 320% increase in tube diameter to enhance load-bearing capacity. Additionally, amorphous carbon was in situ deposited at CNT junctions to form flexible, energy-dissipating interconnections. This multiscale design strategy effectively breaks the traditional strength–toughness trade-off in carbon aerogels, representing a critical step toward their practical and structural deployment in demanding environments.

#### **Biography:**

Associate Professor at Harbin Institute of Technology, China, specializing in carbon nanotube aerogels for advanced applications. His research spans flexible electronics, energy storage, and lightweight structural materials, with 25 SCI publications in high-impact journals including *Advanced Functional Materials*, *npj Flexible Electronics*, and *Materials Horizons*. He has led multiple projects supported by the National Natural Science Foundation of China.

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## Oral Talk:

### Atomic Layer Deposition of MoO<sub>2</sub> Thin Films for Next-Generation DRAM Capacitor Electrodes

Kyung Joon Lee<sup>1\*</sup>, Byeong Jun Jeon<sup>1</sup>, Se Eun Kim<sup>1</sup>, Kyeong Hyun Choi<sup>1</sup>, Sang Woon Lee<sup>1</sup>

<sup>1</sup>*Department of Energy System Research and Department of Physics, Ajou University, Gyeonggi-do, 16499, Republic of Korea*

#### Abstract:

As dynamic random-access memory (DRAM) scaling continues, the development of thin films with high dielectric constants becomes critical for maintaining sufficient capacitance while storing data in the capacitor. Perovskite-structured materials such as SrTiO<sub>3</sub> offer significantly high dielectric constants, making them promising candidates for next-generation applications. Unfortunately, deposition of dielectrics on metal electrodes leads to the formation of interfacial dead layers, which results in significantly reduced dielectric constants. One effective strategy to mitigate this is using electrodes with the identical perovskite structure, minimizing lattice mismatch and interfacial defects.

In this work, the atomic layer deposition (ALD) of MoO<sub>2</sub> thin films was investigated to develop a perovskite SrMoO<sub>3</sub> electrode. A new precursor (based on amidinate ligands) was evaluated for the deposition of MoO<sub>2</sub> thin films using O<sub>2</sub> as the reactant.

The deposited MoO<sub>2</sub> thin films were characterized using four-point probe measurements, X-ray photoelectron spectroscopy (XPS), and X-ray diffraction (XRD). Electrical resistivity measurements showed that the MoO<sub>2</sub> electrode exhibited lower resistance compared to previous studies, demonstrating its potential as a high-performance electrode material.

XPS analysis confirmed a dominant Mo<sup>4+</sup> oxidation state with low C impurity levels in the MoO<sub>x</sub> thin films, with the formation of a polycrystalline MoO<sub>2</sub> phase. These results highlight the potential of ALD-grown MoO<sub>2</sub> films as high-performance electrodes for advanced DRAM capacitor applications.

#### Biography:

Kyung Joon Lee is a master's student in the Department of Physics and the Department of Energy Systems Research at Ajou University, Republic of Korea. He is currently conducting research under the supervision of Professor Sang Woon Lee. His work focuses on the atomic layer deposition (ALD) of thin films, particularly MoO<sub>2</sub>, for next-generation DRAM capacitor electrode applications. His research interests include thin film growth, material characterization, and high-k dielectric integration for advanced semiconductor devices.

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## Poster Presentation

### Hierarchical, flower-like, nanostructured layers of biophenols as green corrosion inhibitors

*Regina Fuchs-Godec*<sup>\*</sup>

*University of Maribor / Faculty of Chemistry and Chemical Engineering, Slovenia*

#### **Abstract:**

The significant economic and environmental impact of metal corrosion has intensified scientific efforts to develop sustainable protection strategies. Current research trends emphasize green approaches, the promotion of environmentally friendly inhibitors, and consideration of the circular economy principle of "waste as raw material." In this study, the copper surface was functionalized with stearic acid, a naturally occurring saturated fatty acid, to increase the hydrophobicity of a self-assembled biophenolic layer. Rosehip oil extract, which is rich in phenolic acids and flavonoids, served as the main source of bioactive molecules that support surface adhesion and antioxidant protection. The self-assembly process led to the formation of hierarchical, flower-like microstructures consisting of nanostructured petal-like elements that act as an effective corrosion barrier. The corrosion inhibitory effect of the hydrophobic layer on copper was evaluated by electrochemical impedance spectroscopy and potentiodynamic polarization in acidic solutions (pH 1–5) simulating acidic urban rain. The self-assembled layers were prepared by immersing copper in various concentrations of rosehip extract dissolved in an ethanolic solution of 0.05 M stearic acid. The electrochemical results showed that stearic acid coating alone has limited stability in acidic media (inhibition effect ~72 % at pH =1). However, the addition of rosehip extract significantly improved the corrosion resistance and increased the inhibition effect to over 94 %. These results demonstrate the potential of natural bioactive compounds in combination with fatty acids for the development of green, sustainable corrosion protection systems.

#### **Biography:**

Prof. Dr. Regina Fuchs-Godec is a professor at the University of Maribor, Slovenia. Her research focuses on surface chemistry, corrosion protection, and green corrosion inhibitors.

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## Poster Presentation

### Acoustic and optical responses of hollow Au nanoparticles to femtosecond laser irradiation

*Behnoush Khammar<sup>1\*</sup>, Ovidio Peña-Rodríguez<sup>2</sup>, Juan A. Monsoriu<sup>1</sup>, Pedro Fernández de Córdoba<sup>3</sup>, and Juan Carlos Castro-Palacio<sup>1</sup>*

<sup>1</sup>*Centro de Tecnologías Físicas, Universitat Politècnica de València, Valencia, Spain*

<sup>2</sup>*Institute of Nuclear Fusion, Technical University of Madrid, Madrid, Spain*

<sup>3</sup>*Instituto Universitario de Matemática Pura y Aplicada, Universitat Politècnica de València, Valencia, Spain*

#### Abstract:

Hollow metal nanoparticles exhibit unique structural, optical, and catalytic properties, making them highly valuable across various fields. In biomedical applications, they show promise for drug delivery, enabling controlled and targeted release, as well as photothermal therapy, where gold nanoshells absorb near-infrared light and convert it into heat. Additionally, they are used in plasmonic biosensors, bioimaging, and diagnostic applications, leveraging their strong surface plasmon resonance to enhance imaging contrast. In this study, we investigate the acoustic and optical responses of hollow gold nanoparticles (10–50 nm) under femtosecond laser irradiation. Molecular dynamics (MD) simulations are performed using the LAMMPS software, with EAM potentials to model Au-Au interactions. The oscillatory behavior of the hollow particles is characterized by a decrease in their mean radius, following damped oscillations around an equilibrium value, which drives thermal expansion. To further analyze the breathing mode, we compute the hyperradius in hyperspherical coordinates. The optical response is examined across different particle sizes as a function of aspect ratio and wavelength. Notably, the localized surface plasmon resonance (LSPR) position shifts significantly toward the infrared spectrum for larger aspect ratios, which is particularly relevant for certain biomedical applications. Finally, we compare the behavior of hollow nanoparticles with that of solid nanospheres, highlighting key differences in their dynamic and optical properties.

#### Biography:

Behnoush Khammar is a Ph.D. student in Physics at the Polytechnic University of Valencia, Spain. She has more than 10 years of research experience in the field of materials science, with a particular focus on nanomaterials. Her work involves both computational and experimental approaches, combining simulation techniques with laboratory-based studies to explore the structural and functional properties of advanced materials. She has developed skills in modeling, data analysis, and materials characterization. Her research aims to contribute to the development of innovative nanomaterials with potential applications in energy, electronics, and emerging technologies.



## Poster Presentation

### Study of Bio-Based Fillers and Additives for the Production of Biodegradable Biopolymers

Gioele Foltran<sup>1,2</sup>, Silvia Conca<sup>3</sup>, Valentina Beghetto<sup>1,3,4</sup>

<sup>1</sup>*Department of Molecular Sciences and Nanosystems, University Ca' Foscari of Venice, Via Torino 155, 30172 Mestre, Italy*

<sup>2</sup>*Department of Architecture and Industrial Design, University of Campania "Luigi Vanvitelli", Aversa, Italy*

<sup>3</sup>*Crossing S.r.l., Viale della Repubblica 193/b, 31100 Treviso, Italy*

<sup>4</sup>*Consorzio Interuniversitario per le Reattività Chimiche e La Catalisi (CIRCC), Via C. Ulpiani 27, 70126 Bari, Italy*

#### Abstract:

Beer spent grain (BSG), main side-stream of breweries, is an unexploited, costless and widely available resource for the biorefinery. For the first time BSG has been employed as bio-filler (BSGF) with polybutylene succinate (PBS) as polymer matrix, to produce new bio-composites (PBS-BSGF), reducing virgin biomass and fossil-based polymers consumption, transforming waste into a valuable resource. Additionally, BSG can become a valuable resource also for the production of biobased compatibilizers. Generally, bio-composites require the use of additives, commonly fossil based, to improve compatibility between the polymer (apolar) and the filler (polar). BSG lipid component can be chemically modified to obtain hydrophilic-hydrophobic molecules able to enhance the compatibility polymer/filler. Initially, oleic acid and linoleic acid were chosen as model compounds to synthesise different potentially efficient additives by esterification, and epoxidation<sup>1-3</sup>. Subsequently, the lipid component was extracted with organic solvents from BSG and esterified, epoxidized. All additives were characterized by NMR, FT-IR, and elemental analysis. Different PBS/BSG composites formulations were prepared with and without additives to verify their efficiency by DSC, ATR, and TGA.<sup>4</sup>

This work represents the first example of valorisation of an agrifood waste both as filler and as compatibilizer for the production of biodegradable composites.

#### Biography:

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## Poster Presentation

### Structure and morphology of hydrothermally synthesized Sm-doped ceria

Kolyo Kolev<sup>1\*</sup>, O. Dimitrov<sup>1</sup>, G. Avdeev<sup>2</sup>, M. Dimitrova<sup>1</sup>, T. Petkova<sup>1</sup>

<sup>1</sup>*Institute of Electrochemistry and Energy Systems, Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl.10, Sofia, 1113, BULGARIA;* <sup>2</sup>*Institute of Physical Chemistry, Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl.11, Sofia, 1113, BULGARIA;*

#### Abstract:

The main topic of this work is to investigate the structure, morphology and basic physical-chemical properties of samarium-doped ceria ( $\text{Ce}_{1-x}\text{Sm}_x\text{O}_{2-x/2}$ , ( $x = 0, 0.1, 0.2, 0.3, 0.4$  and  $0.5$ )) using the hydrothermal method of synthesis. The use of hydrothermal synthesis (HdT) lies in its numerous advantages as an economical, environmentally friendly and low-emission method for synthesis which are needed nowadays. Samples of  $\text{Ce}_{1-x}\text{Sm}_x\text{O}_{2-x/2}$ , ( $x = 0, 0.1, 0.2, 0.3, 0.4$  and  $0.5$ ) were synthesized by hydrothermal synthesis and were washed, dried and calcined. The phase composition, morphology, homogeneity, crystallinity, structural units, specific surface area and size of the particles were examined with multiple analysis methods such as XRD, SEM/EDX, Raman, FTIR, BET.

#### Biography:

**Kolyo Kolev**, PhD, is a Chief Assistant Professor at the Institute of Electrochemistry and Energy Systems (IEES), Bulgarian Academy of Sciences. He holds BSc and MSc degrees in Semiconductor Technology and Materials, and a PhD in physical-chemistry. His research focuses are on the synthesis and physical and physical-chemical characterization of rare-earth and transition metal oxides for electrochemical applications, including thin films. Dr. Kolev has received several awards, including a DAAD scholarship and recognition as “Most Prosperous Young Scientist” of the IEES, BAS (2009).

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## **Poster Presentation**

### **Graphene oxide as a support for the active components of the catalyst**

Darja Pečar\*, Andreja Goršek

*Faculty of Chemistry and Chemical Engineering, University of Maribor, Smetanova 17, 2000  
Maribor, Slovenia*

#### **Abstract:**

Chemical processes generate large quantities of waste every day. The use of large quantities of reagents generates unwanted by-products. Some chemical processes can be replaced by more efficient catalytic processes that use less energy and fewer necessary components - reagents. Catalyzed reactions mean greener chemistry and greener chemical processes. To ensure a cleaner environment with less waste, chemical processes can be carried out with heterogeneous catalysts (solid active components) instead of homogeneous catalysts (e.g. acids or bases), which can be easily removed from the reaction medium after completion of the reaction and can also be reused several times.

Graphene oxide as a catalyst support has many advantages due to its unique structure and chemical properties. It has a large specific surface area and contains various oxygen functional groups. Compared to conventional catalyst supports such as activated carbon or metal oxides, graphene oxide is more environmentally friendly. It is synthesized from cheap graphite and is recyclable, so we think it is a better choice.

In this study, graphene oxide was synthesized and served as a catalyst support. We bound the active components to the resulting support. The synthesized catalysts were characterized by N<sub>2</sub> adsorption, scanning electron microscopy, temperature-programmed desorption, Fourier transform infrared spectroscopy and X-ray fluorescence spectroscopy. Based on the characterization results, we selected the most efficient catalysts to perform model reactions of fructose dehydration under different experimental conditions. The resulting products were analyzed by HPLC and the conversion was subsequently calculated.

#### **Biography:**

Dr. Darja Pečar received her M.Sc. and Ph.D. degrees from the Faculty of Chemistry and Chemical Engineering University of Maribor in 2002 and 2005, respectively. She is an associate professor at the Faculty of Chemistry and Chemical Engineering University of Maribor. Her teaching activities cover the fields of bioreaction engineering, chemical reaction engineering and materials. Her research activities include the synthesis of chemical and biochemical catalysts, kinetic studies of chemical and biochemical reactions and safety studies in the pharmaceutical industry.

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## Poster Presentation

### Surface Engineering of Metal Powders: Scalable Modification via Fluidized Bed Processing

*Neyder A. Sandoval<sup>1</sup>\* Sergio Sánchez Delgado<sup>2</sup>; Daniel Serrano Garcia<sup>2</sup>, Sophia A. Tsipas<sup>1</sup>*

*<sup>1</sup> Materials Science and Engineering Department, IAAB, Universidad Carlos III de Madrid, Avda. Universidad 30, 28911, Leganes, Madrid, Spain*

*<sup>2</sup> Department of Thermal and Fluid Engineering, Universidad Carlos III de Madrid, Avda. Universidad, 30, 28911, Leganes, Madrid, Spain*

#### **Abstract:**

In the pursuit of improving powder properties for additive manufacturing (AM), surface modification of metal powders emerges as a promising solution. This work focuses on the development of a scalable and cost-effective process for modifying the surface of Al2024 powder using a custom-designed fluidized bed system. The system enables homogeneous coating of micrometric particles with selected nanoparticles (e.g., TiC, SiC, LaB<sub>6</sub>) without affecting the morphology, particle size, or flowability critical to laser powder bed fusion (LPBF) processes.

Our approach addresses limitations observed in conventional surface modification techniques—such as mechanical mixing or wet chemical methods—which often face challenges in scalability, reproducibility, or result in unwanted phase transformations. By utilizing a fluidized bed process operated at controlled conditions and mild temperatures, we successfully deposit nanoparticulate coatings while preserving powder integrity and avoiding issues associated with high-temperature treatments.

This tailored surface modification has shown potential for enhancing laser absorption, thermal conductivity of the feedstock, ultimately contributing to the elimination of microstructural defects such as cracking and porosity during LPBF of Al2024 alloys. The approach is also adaptable to other metal powder systems, paving the way for broader application in AM industries.

The poster presents the process design, characterization of modified powders, and a comparative analysis of surface properties and flowability against unmodified powders, demonstrating a pathway towards more reliable and cost-efficient AM feedstocks.

#### **Biography:**

I am a third-year Ph.D. student in Materials Science and Engineering, with an academic background in Industrial Engineering and a Master's degree in Materials Science and Engineering. My research focuses on the development of surface modification processes for metallic powders intended for additive manufacturing applications, with an emphasis on

optimizing aluminum alloy processing via Laser Powder Bed Fusion (LPBF). My work includes the design and implementation of innovative experimental systems for powder functionalization and the integration of advanced laser profiles to enhance microstructural integrity in printed components. I aim to contribute to the advancement of scalable, cost-effective solutions for next-generation additive manufacturing technologies.

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## Poster Presentation

### **Photo-degradation of organic dye mixtures and ciprofloxacin antibiotic utilizing spray deposited Li-Nb co-doped SnO<sub>2</sub> thin films**

*Gouranga Maharana<sup>1\*</sup>, Yuvashree Jayavelu<sup>1</sup>, D Paul Joseph<sup>1</sup>*

*<sup>1</sup>Department of Physics, National Institute of Technology, Warangal, Telangana State, 506004, India.*

#### **Abstract:**

Spray-coated SnO<sub>2</sub> thin films with Nb and Li as co-dopants have been utilized as a transparent conducting photoelectrode for the photodegradation of organic contaminants. X-ray diffraction demonstrates successful doping of 'Nb' and 'Li' into the SnO<sub>2</sub> lattice, resulting in highly textured growth along the (110) plane direction. FESEM micrographs show that tetragonal-shaped particles (0 - 1 wt.% Li doped Nb (2 wt.%): SnO<sub>2</sub>) agglomerate mildly, generating more slender grains (2 - 4 wt.% Li doped Nb (2 wt.%): SnO<sub>2</sub>). The wettability of the films as determined by contact angle measurement, suggests that they are hydrophilic in nature. Nb and Li codoping into the SnO<sub>2</sub> lattice improves transmittance from 53% for pure to 72% for 4 wt.% Li and 2 wt.% Nb codoped SnO<sub>2</sub> thin films. The linear four-probe and Hall effect demonstrated sheet resistance and electrical transport qualities with a minimal sheet resistance of 56  $\Omega/\square$  and the highest mobility of 34.75 cm<sup>2</sup> V<sup>-1</sup>s<sup>-1</sup> for 4 wt.% Li and 2 wt.% Nb doped SnO<sub>2</sub> thin films, respectively. Based on the assessed optoelectronic properties, the photocatalytic study for solely methyl violet, mixed dyes (malachite green, methyl orange, and methylene blue), and ciprofloxacin antibiotic degradation has been performed using the optimal film, and significant degradation efficiency was attained under both sunlight and low powered LED light illumination. These results will be presented and discussed in detail.

#### **Biography:**

Myself Gouranga Maharana, a research scholar pursuing a Ph.D. at the Dept of Physics, National Institute of Technology in Warangal, India. My current research is on spray coating of oxide thin films to test them as immobilized electrodes for photo-catalysis for low-power and inexpensive dye degradation. I have currently published two first-author papers in Surfaces and Interfaces (Elsevier), one in Chemistry Select (Wiley), and one is under review in Bulletin of Materials Science (Springer).

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## Poster Presentation

### A Transformer-Based Discontinuity Detection Method for Numerical Simulation of Porous Materials

*Jiaqian Dan<sup>1,\*</sup>, Jiebao Sun<sup>1</sup>, Jia Li<sup>1</sup>*

*<sup>1</sup> Harbin Institute of Technology, China*

#### **Abstract:**

Porous materials are widely used in energy devices, environmental systems, and biomedical applications due to their multiscale structures and exceptional physicochemical properties. However, during service, they often exhibit discontinuous behaviors such as pore collapse, microcrack propagation, and interfacial damage, which critically affect performance and durability. Accurate and efficient identification of these discontinuities is essential for reliable numerical simulation and design. This study proposes a Transformer-based discontinuity detection method tailored for complex material responses. High-order Discontinuous Galerkin (DG) solutions are used to construct physically meaningful jump indicators, which are fed into a Transformer model. Exploiting its strong sequence modeling and global attention capabilities, the model classifies computational cells as “smooth” or “discontinuous.” For the latter, a high-order Weighted Essentially Non-Oscillatory (WENO) reconstruction is applied to improve local accuracy and stability, while DG maintains its efficiency in smooth regions. The method operates in an offline inference mode, offering scalability and adaptability. Applied to carbon-based porous materials such as carbon aerogels and graphene foams, it outperforms traditional TVD limiters and conventional neural networks (e.g., CNNs, MLPs) in accuracy, robustness, and generalization. This work provides a robust and generalizable simulation strategy for porous material modeling across energy, environmental, and biomedical domains, and promotes the integration of advanced AI models like Transformers into computational materials science.

#### **Biography:**

Jiaqian Dan is a Ph.D. candidate at Harbin Institute of Technology, specializing in neural networks and intelligent modeling of complex materials. Her research focuses on integrating machine learning with numerical simulation to address multiscale and discontinuous phenomena in porous materials. In particular, she applies physics-informed neural networks (PINNs) to tackle challenging problems across biomechanics, mechanics, and materials science.

## Poster Presentation

### Phosphorous doped Si Nanowires for High-Capacity Battery Anodes and High-Power Supercapacitors

Rashmi Tripathi<sup>1,2</sup>, Sumana Kumar<sup>2\*</sup>, Amartya Mukhopadhyay<sup>2</sup>, Rajiv O. Dusane<sup>1</sup>

<sup>1</sup> *Semiconductor Thin Films and Plasma Processing Laboratory, Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Powai, Mumbai 400076, India*

<sup>2</sup> *Advanced Batteries and Ceramics Laboratory, Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Powai, Mumbai 400076, India*

#### Abstract:

This study addresses the challenges of poor cyclic stability and modest rate-capability in stand-alone Si-based anodes for Li-ion batteries by developing phosphorus-doped n-type silicon nanowires (SiNWs) directly grown on Cu current collectors via a single-step hot wire-assisted vapor-liquid-solid method. By varying phosphine concentration during synthesis, uniform doping of both crystalline-Si core and amorphous-Si shell regions is achieved, with increased dopant content altering SiNW morphology from “grass-like” to “solid tube-like” structures while enhancing amorphous phase content. Electrochemical evaluations as Li-ion battery anodes reveal that optimized phosphorus doping significantly improves performance: a delithiation capacity of ~2916 mAh/g at 1C rate is retained at ~94% after 100 cycles, demonstrating exceptional cyclic stability. Rate-capability tests show ~53% retention of initial capacity (at C/5) even at 5C, surpassing conventional Si-based anodes. As supercapacitor electrodes, phosphorus-doped SiNWs exhibit an areal capacitance of ~847 mF/cm<sup>2</sup> at 5 mV/s, ~6.5 times higher than undoped counterparts (131 mF/cm<sup>2</sup>). Symmetric supercapacitor cells deliver an areal energy density of 0.26 mWh/cm<sup>2</sup> at 3.17 mW/cm<sup>2</sup>, outperforming most reported Si-based devices. This work establishes a facile route for synthesizing tunable n-type SiNWs and provides a correlative understanding of how dopant concentration influences morphology, crystallinity, and electrochemical behavior. The dual applicability of phosphorus-doped SiNWs in high-energy Li-ion batteries and high-power supercapacitors underscores their versatility for advanced energy storage systems, offering pathways to address critical limitations of Si-based materials in next-generation devices.

#### Biography:

Dr. Sumana Kumar is currently an Institute Postdoctoral Fellow at the Department of Metallurgical Engineering and Materials Science, IIT Bombay, India. She received her Ph.D. in Instrumentation and Applied Physics, focusing on advanced supercapacitor systems. Her research spans solid-state lithium batteries, polymer-ceramic composite electrolytes, anode-

less batteries, and hybrid energy storage devices. Her work integrates material design, electrochemical analysis, and energy conversion technologies for next-generation energy storage.

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## **Poster Presentation**

### **Development of a Power Generator Based on a Snap-Action Bistable Structure and Shape Memory Alloy Springs**

Pan Chi Hsiang

*Department of mechanical engineering, National Chin-Yi university of technology, Taiwan  
(R.O.C)*

#### **Abstract:**

A large amount of waste heat in the form of low temperature is generated during the operation of industrial production processes or machinery and equipment. Low-temperature waste heat offers great potential for work because it exists in abundance around us, but there is a lack of effective methods by using low-temperature heat to generate electricity. The collection and utilization of low-temperature waste heat is very contributing to the carbon neutral process and environmental impact, which is in line with innovative energy and efficient use of waste energy. In this paper, a power generator based on a bistable structure and shape memory alloy springs is developed for thermal to electric conversion. The construction of the power generator can be divided into three main parts: (1) thermal actuating mechanism with a bistable structure and shape memory alloy springs; (2) hot and cold fluidic sources circulation conduits; (3) electric generation motor. The snap-action of the bistable structure is done by utilizing thermal actuation of the shape memory alloy springs, which are performed by hot and cold fluidic sources circulation conduits. When sufficient force from the shape memory alloy springs is applied at the bistable structure, the snap-through of the bistable structure from one stable position to another can strongly pull or push the electric generation motor to rotate rapidly. We have studied some factors that strongly affect the performance of the thermal actuating mechanism. A prototype of power generator is demonstrated for previous testing. The power generation can be applied to a wide range of heat sources, including: waste heat from machinery and equipment and industrial output, or from natural heat sources. Compared with power generation with the thermoelectric material technology, the power generation is more applicable to low-temperature heat sources, or heat sources with low temperature gradients.

#### **Biography:**

Chi Hsiang Pan is a professor in Department of Mechanical Engineering, National Chin-Yi University of Technology, Taiwan, ROC. He obtained the PhD degree in mechanical



engineering from the Department of Mechanical Engineering at National Chiao Tung University. He majored in mechanical, microelectromechanical, and mechatronic research. He has served as the chief secretary, dean of students, academic and general affairs, etc. He also served as the director of the Institute of Precision Mechanical Engineering.

## Poster Presentation

### **An *Artemisia sphaerocephala* Krasch-based Food-grade Superabsorbent Polymer for Food Industrial Applications**

*Nathanael Chun Him Lai<sup>1,2\*</sup>, Xinwei Xu<sup>1,2</sup>, Hao Wu<sup>1,2</sup>*

*<sup>1</sup>Department of Food Science and Nutrition, The Hong Kong Polytechnic University, Hung Hom, Hong Kong, China*

*<sup>2</sup>Research Institute for Future Food, The Hong Kong Polytechnic University, Hung Hom, Hong Kong, China*

#### **Abstract:**

In light of the ongoing interest in sustainable development and green manufacturing, it is highly significant to develop new bio-based sustainable materials to replace synthetic materials. Synthetic polymer-based superabsorbent polymers (SAP) such as polyacrylates, polyacrylamides, and maleic anhydride copolymers have been extensively used in various applications, including disposable hygiene products, spill control, food packaging, and agricultural use. However, synthetic superabsorbent polymers are generally non-biodegradable and toxic, which poses an environmental and safety concern. Therefore, it is of high importance to develop a sustainable, food-based superabsorbent polymer.

Herein, we report the preparation of *Artemisia sphaerocephala* Krasch (ASK)-based superabsorbent polymers via esterification of ASK with green crosslinkers and subsequent polymerization with minimal acrylic acid (AA). Fourier transform infrared spectroscopy (FTIR) confirmed the successful synthesis of ASK-SAP. By fine-tuning the esterification degree of ASK and esterified ASK: AA ratio, the as-prepared ASK-SAP exhibited excellent water absorbency (over 900 g absorbed water/g food-based SAP), and elicited better swelling properties and absorption of saline when compared with synthetic SAP poly(acrylic acid) (PAA). Scanning electron microscopy (SEM) analysis revealed the porous structure of esterified ASK and ASK-SAP, which indicates that the ASK esterification is crucial to create well-defined three-dimensional polysaccharide networks for enhanced water absorption. We envision this novel series of food-based SAP as instrumental in food industrial applications and promoting the use of food-based materials for sustainable development.

**Biography:**

Dr. Lai's research group focuses on developing food-based materials for biomedical and agricultural applications and on developing new methods for sustainable and green manufacturing. He has published 15 peer-reviewed top journals and 2 patents, including *ACS Nano*, *Advanced Materials*, and *Carbohydrate Polymers*. He has also been a registered European Commission expert since 2023.

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## Day 3, Room A

### Invited Talk

#### **Numerical strategies to enhance the use of topologically optimised designs with real load and material conditions, and a stiffness-volume space to perform AI-accelerated designs**

*Luis Saucedo Mora*

##### **Abstract:**

In the automotive and aerospace industries, the need for optimised structures offering the best mechanical performance for the minimum weight is ubiquitous. To that aim, Topology optimization (TO) is a very popular structural design tool. Particularly, the Solid Isotropic Material with Penalization (SIMP) method offers a trade-off between minimum compliance (i.e., maximum stiffness) and a fixed amount of material for a given set of static, deterministic boundary conditions. Since TO is a non-convex problem, its gradient can be tuned by filtering the topology's contour, creating sharper material profiles without necessarily compromising optimality. However, despite simplifying the layout, some filters fail to address manufacturability concerns such as capillarity (thin tweaks as struts) generated by uncertain loading, vibration, or fatigue. A tailored density-based filtering strategy is offered to tackle this issue. Additionally, volume fraction is left unconstrained so material can be strategically replenished through a logarithmic rule acting on the updated compliance. In doing so, an interpolation space with three degrees of freedom (volume, compliance, minimum thickness) is created, yielding diverse topologies for the same boundary conditions and design values along different stages of evolving topological families with distinct features.

##### **Biography:**

Luis Saucedo Mora is an active researcher in the field of experimental and computational solid mechanics, with international experience at different universities. In 2019, he became a senior lecturer at the Polytechnic University of Madrid at the School of Aerospace Engineering. He has co-authored different patents and software registers, as well as published more than 40 JCR research papers in collaboration with more than 20 different institutions worldwide.

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## Invited Talk

# Obtaining polypyrrole from Biomass Catalytic Pyrolysis and Their Application in Epoxy Resin Composites

*Pamela Hidalgo Oportol and Mauricio Yáñez Sanchez<sup>2</sup>*

*<sup>1</sup>Department of Industrial Processes, Faculty of Engineering, Universidad Católica de Temuco, Rudecindo Ortega 02950, Temuco, Chile.*

*<sup>2</sup>Department of Biological and Chemical Sciences, Faculty of Natural Resources, Universidad Católica de Temuco, Rudecindo Ortega 02950, Temuco, Chile.*

### Abstract:

Polypyrrole (PPy) is an electroconductive polymer belonging to a unique class of materials that combine metallic and semiconductor properties with polymeric characteristics such as flexibility, strength, elasticity, and ease of oxidation. Its high conductivity compared to other polymers, along with the ongoing pursuit of environmentally friendly synthesis processes, makes it a promising material. However, one of the main challenges in its development lies in the conventional synthesis methods, which are highly polluting.

This study presents an alternative, environmentally friendly route for PPy synthesis. The process consists of two steps: (1) In situ catalysis of lignocellulosic biomass in an ammonium atmosphere to obtain pyrrole (Py), and (2) oxidative polymerization of Py. The study analyzed key parameters influencing Py formation via thermochemical processes, including temperature, biomass particle size, and catalyst-to-biomass weight ratio. The oxidative polymerization of Py was then carried out, evaluating the effects of different doping and oxidizing agents on the renewable-based PPy. Finally, the PPy-epoxy resin composite was synthesized and characterized in terms of its chemical, thermal, electrical, and mechanical properties.

### Biography:

Pamela Hidalgo completed her doctoral and postdoctoral studies at the Universidad de La Frontera in Temuco. She is currently a faculty member in the Department of Industrial Processes at the Catholic University of Temuco. She has published over 20 articles in renowned journals and has been awarded scientific research grants, including Fondecyt No. 11221146.

Mauricio Yáñez earned his doctorate at the Universidad de Santiago de Chile. He is a faculty member in the Department of Biological and Chemical Sciences, Faculty of Natural Resources, at the Catholic University of Temuco. He has published more than 25 articles in prestigious journals and has received scientific research grants, including Fondecyt Regular.

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## Oral Talk

### **Magnetic NiFe<sub>2</sub>O<sub>4</sub>-PVDF Composites: Combining Flexibility, Stability, and Superior Magnetic Properties for Functional Applications**

*Sarah BAAYYAD<sup>1</sup>, Chaymae BAHLOUL<sup>1</sup>, Fatima-Zahra SEMLALI<sup>1</sup>, El Kébir HLIL<sup>3</sup>, Tarik MAHFOUD<sup>2</sup>, Hassan EL MOUSSAOUI<sup>2</sup>, Mounir EL ACHABY<sup>1</sup>*

*<sup>1</sup> Materials Science, Energy and Nanoengineering Department (MSN), Mohammed VI Polytechnic University (UM6P), Lot 660 – Hay Moulay Rachid, 43150, Ben Guerir, Morocco.*

*<sup>2</sup> Moroccan Foundation for Advanced Science, Innovation and Research (MASCIR), Rabat Design Center, Rue Mohamed El Jazouli, Madinat El Irfane, 10100 Rabat, Morocco.*

*<sup>3</sup> Institut Néel, CNRS et Université Joseph Fourier, BP 166, F-38042 Grenoble cedex 9, France.*

#### **Abstract:**

In this study, magnetic flexible polymer composite films with enhanced magnetic properties were successfully developed, targeting advanced applications such as electromagnetic interference (EMI) shielding. Initially, a practical method was employed to synthesize NiFe<sub>2</sub>O<sub>4</sub> nanoparticles with controlled particles sizes. Magnetic characterization revealed that the synthesized nanoparticles exhibit superparamagnetic behavior with a saturation magnetization of 57.80 emu/g and an average particle size of 26.733 nm. Subsequently, a high concentration magnetic composite film was fabricated by integrating nickel ferrite nanoparticles into a poly(vinylidene fluoride) (PVDF) matrix. The resulting composite films demonstrated remarkable flexibility, excellent thermal stability, and superior magnetic performance, making them highly suitable for EMI shielding applications. These findings highlight the potential of such composite materials for multifunctional applications in advanced technologies.

#### **Biography:**

Sarah baayyad , Ph.D Student.

Sarah Baayyad, is currently a PhD student at Materials Science and Nanoengineering department –Mohammed VI Polytechnic University– Benguerir- Morocco. She received in 2021 her master's degree in functional materials and additive manufacturing. She is currently working on the development, fabrication and characterization of high-performance polymer magnetic composite materials based on thermoplastic polymers

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## Oral Talk:

### **Biocompatible BCZT Core@CuFe<sub>2</sub>O<sub>4</sub> Shell Structure Embedded in PVDF Matrix: A Sustainable Approach for High-Efficiency Magnetoelectric Energy Harvesting**

*Chaymae BAHLOUL<sup>1, \*</sup>, Sarah Baayad<sup>1</sup>, Adil EDDIAI<sup>2</sup>, Omar CHERKAoui<sup>3</sup>,  
M'hammed Mazraoui<sup>2</sup>, Fatima-Zahra SEMLALI<sup>1</sup>, Mounir EL ACHABY<sup>1</sup>*

*<sup>1</sup>Materials Science, Energy and Nanoengineering Department (MSN), Mohammed VI Polytechnic University (UM6P), Lot 660 – Hay Moulay Rachid, 43150 Ben Guerir, Morocco*

*<sup>2</sup>Laboratory of Physics of Condensed Matter (LPMC), Faculty of Sciences Ben M'Sik, Hassan II University, Casablanca, Morocco*

*<sup>3</sup>REMTEX Laboratory, Higher School of Textile and Clothing Industries (ESITH), Casablanca, Morocco*

#### **Abstract:**

In the pursuit of sustainable and high-performance magnetoelectric materials, we report the design and fabrication of a novel nanocomposite consisting of biocompatible Ba<sub>0.8</sub>Ca<sub>0.2</sub>Zr<sub>0.1</sub>Ti<sub>0.9</sub>O<sub>3</sub> (BCZT) core@CuFe<sub>2</sub>O<sub>4</sub> (CFO) shell structures uniformly embedded within a poly (vinylidene fluoride) (PVDF) matrix. These core-shell structures were synthesized via a tailored hydrothermal-assisted route, enabling precise control over morphology and interface characteristics. The optimized architecture promotes efficient ferroelectric-ferromagnetic coupling at the nanoscale, crucial for enhancing magnetoelectric effects. Comprehensive characterization using XRD, FTIR, and STEM confirms the successful formation of well-defined core-shell structures and their homogeneous dispersion in the PVDF matrix. Notably, a substantial increase in  $\beta$ -phase content was observed (93%), contributing to improved piezoelectric response and dielectric properties. The resulting flexible nanocomposite films exhibit strong magnetoelectric coupling, excellent flexibility, and reliable performance under mechanical deformation and ambient variations. This work demonstrates a sustainable and scalable strategy for engineering multifunctional polymer nanocomposites by employing earth-abundant, non-toxic constituents, paving the way for advanced applications in self-powered biomedical implants, smart textiles, structural health monitoring, and wearable electronics. The integration of biocompatibility with energy harvesting efficiency marks a significant step toward the development of next-generation flexible electronics

**Keywords:** Core-shell structures, BCZT, CuFe<sub>2</sub>O<sub>4</sub>, PVDF, magnetoelectric coupling,  $\beta$ -phase, piezoelectric, energy harvesting, flexible electronics, biocompatible composites

#### **Biography:**

**Chaymae Bahloul** is a third-year PhD student in the Polymer & Composites (PolyCom) team at **Mohammed VI Polytechnic University** (UM6P), Morocco. Her research focuses on the development and characterization of electroactive PVDF-based nanocomposites, enhanced with functional nanoparticles such as phosphate and ferrite fillers with biocompatibility. These materials aim to improve energy harvesting efficiency for applications in flexible electronics and autonomous systems.

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## Oral Talk

### Advanced Reaction Pathways in the Atomic Layer Deposition of TiN Thin Films for Reduced Resistivity

*Kyeong Hyeon Choi<sup>1\*</sup>, Se Eun Kim<sup>1</sup>, Byeong Jun Jeon<sup>1</sup>, Kyeong Jun Lee<sup>1</sup>, Sang Woon Lee<sup>1</sup>*

*Department of Physics / Department of Energy Systems Research, Ajou University, Republic of Korea*

#### Abstract:

Titanium nitride (TiN) thin films grown by atomic layer deposition (ALD) are widely studied as electrode materials for semiconductor devices, such as logic transistors and dynamic random access memories (DRAMs).  $\text{TiCl}_4$  and  $\text{NH}_3$  are typically used as Ti and nitrogen precursors in the TiN ALD process. However, the resistivity of TiN films increases at lower deposition temperatures, particularly below 400 °C, due to residual chlorine impurities (>3%) from  $\text{TiCl}_4$ . Generally, a process temperature higher than 500 °C is necessary to achieve a low resistivity of the TiN film.

In this work, we propose an advanced ALD process using a novel surface reaction route to reduce film resistivity at lower temperatures that are low enough to prevent transistor degradation. By introducing HBr after the  $\text{TiCl}_4$  pulse, titanium bromide is temporarily formed and subsequently converted into TiN by subsequent  $\text{NH}_3$  injection. HBr induces the substitution of Br for Cl, weakening the strong Ti–Cl bonds and forming Ti–Br bonds, effectively removing Cl from the Ti surface. This modified process resulted in a >20% reduction in resistivity compared to the conventional  $\text{TiCl}_4 + \text{NH}_3$  process at the same temperature ( $\sim < 400$  °C). This is because the Cl concentration in the TiN film was significantly lowered to  $\sim < 1\%$  due to the effect of HBr during surface reactions. The reduced resistivity enables lower power consumption in DRAM operations and allows more aggressive scaling of capacitors for high-density integration. This study provides a promising approach for improving TiN film quality in low-temperature ALD processes.

## Biography

Kyeong Hyeon Choi is currently M.S. student at Ajou University.

Kyeong Hyeon Choi is currently conducting research on atomic layer deposition (ALD) of nitride-based electrodes, perovskite-structured electrodes, and high-k dielectric materials.

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## Invited Talk

### **The effects of pore channel features on the fatigue performances of selective laser melted Dievar mold steel**

*Ming-Wei Wu<sup>1\*</sup>, Zih-Sin Shih<sup>1</sup>, Ming-Hsiang Ku<sup>1</sup>, Xue-Jun Zhuang<sup>1</sup>, Chien-Lun Li<sup>2</sup>*

*<sup>1</sup>Department of Materials and Mineral Resources Engineering, National Taipei University of Technology, Taiwan;*

*<sup>2</sup>voestalpine Technology Institute (Asia) Co., Ltd., Taiwan*

## Abstract:

Selective laser melting (SLM) is the major process of additive manufacturing metallic materials. SLM Dievar mold steel has been applied in commercial molds with conformal cooling channels. However, the influences of pore channel features on the fatigue performance of SLM Dievar steel have not been clarified yet. Thus, the objective of this study was to investigate the roles of pore channel features on the fatigue performance of SLM Dievar steel. Three types of U-notch geometries were used to simulate the effects of pore channel. The results of tensile fatigue tests indicate that the presence of U-notch slightly lowered fatigue limit. However, different U-notch geometries did not lead to a significant fatigue limit variations. The surface condition and roughness were measured using scanning electron microscope in combination of laser scanning microscope. The results show that the downskin area exhibited the higher surface roughness than the upskin area did. Because the surface roughness on the samples with the three types of U-notches were comparable, the features of pore channel investigated in this study did not obviously affect the fatigue properties. This findings was advantageous to the design of SLM mold with conformal cooling channels in the future.

## Biography:

Prof. Ming-Wei Wu is a distinguished professor in the Department of Materials and Mineral Resources Engineering, National Taipei University of Technology, Taiwan. Prof. Wu earned his PhD in Materials Science and Engineering at National Taiwan University in 2007. His areas of expertise include powder metallurgy, additive manufacturing, microstructural characterization, mechanical properties, and fracture analysis. Prof. Wu has published more than 100 articles (journal and conference), including 9 papers in Materials Science and Engineering A, 6 papers in Metallurgical and Materials Transactions A, and 3 papers in



## Oral Talk

### Construction of Perovskite Heterostructures for Next-Generation DRAM Capacitor Fabrication via Atomic Layer Deposition

*Se Eun Kim<sup>1\*</sup>, Byeong Jun Jeon<sup>1</sup>, Kyeong Hyeon Choi<sup>1</sup>, Kyung Joon Lee<sup>1</sup> and Sang Woon Lee<sup>1</sup>*

*<sup>1</sup>Department of Energy System Research and Department of Physics, Ajou University, Gyeonggi-do, 16499, Republic of Korea.*

#### Abstract :

As the density of dynamic random-access memories (DRAMs) continues to increase, cell capacitance inevitably decreases, leading to data read failures. Therefore, innovations in both capacitor structures and high-k/electrode materials are essential. enhance the effective surface area, the adoption of high-k dielectric materials is ultimately essential to meet the capacitance requirements.

Perovskite-structured materials are particularly promising due to their high dielectric constants arising from strong ionic polarization. Among them, SrTiO<sub>3</sub> (STO) stands out with a dielectric constant of approximately 300. However, the formation of a low-k interfacial layer between the dielectric and electrode—known as the dead layer effect—remains a critical limitation. Using an electrode with the same perovskite structure as the dielectric can effectively reduce the dead layer effect at the dielectric/electrode interface.

In this study, we demonstrate the successful fabrication of an in-situ crystallized STO thin film on an SVO electrode using atomic layer deposition (ALD). The perovskite-structured SrVO<sub>3</sub> (SVO) exhibits metallic conductivity due to its V 3d electrons and is structurally compatible with STO. Through careful interface control enabled epitaxial growth of STO on the SVO electrode was achieved, resulting in high crystallinity without the need for post-annealing. The use of perovskite-structured electrodes suppressed the formation of a dead layer at the high-k/electrode interface, leading to a 40% increase in the permittivity of STO.

This work aims to realize an all-perovskite MIM capacitor (SVO/STO/SVO) structure with enhanced dielectric performance and integration potential for next-generation DRAM applications.

#### Biography:

Se Eun Kim is a Ph.D. candidate at the Department of Physics and Energy Systems, Ajou University, South Korea, advised by Professor Sang Woon Lee. She received her B.S. and M.S. degrees in Physics from Ajou University. Her research focuses on the development of high-k dielectric materials, perovskite-structured electrodes, and advanced atomic layer

deposition techniques for DRAM applications. She is currently working on the fabrication of all-perovskite MIM capacitors and the investigation of interfacial phenomena affecting dielectric performance.

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**Oral Talk**  
**Physical and Mechanical Properties of Pumice and Clay Reinforced**  
**Aluminum**  
**Syntactic Foams Produced By Pressure Infiltration Technique**

*Ibrahim Abdüsselam Tantoglu 1 \*, Ismail Cam Akgün 1 , Ali Göksenli 1*  
*1 Istanbul Technical University, Türkiye*

**Abstract:**

Foam materials are characterized by their porous internal structure. Depending on the porosity structure, they can be open or closed. In the absence of interconnection between the cavities, a closed-cell structure is thus formed. In closed-cell foam materials, internal cavities can be created with different methods. In Syntactic Foam Metals (SFM), which is a composite, the inner cavities are formed by hollow or honeycomb-like spheres. SCMs are preferred today due to their lightness, vibration, and energy-damping potential. In our study, 7075 aluminum was selected as the matrix material, and 2-4 mm sphere pumice and clay were selected as reinforcement materials. Nowadays, SKMs are produced through a variety of methodologies. In our project, SFMs were produced by the pressurized infiltration method. The diameter of the obtained cylindrical SKMs is 30 mm, and the height is 40 mm. Density measurements were applied to the produced SKMs, and Optical Microscope analyses were performed to examine their internal structures. Quasi-static compression tests were carried out to determine fracture characteristics of SKMs and significant mechanical properties such as energy absorption capacity, plateau, and compression strength values. To investigate the effects of ceramic sphere material on the density, internal structure, and mechanical properties of SKMs, three different types of SKMs consisting of 100% Pumice, 100% Clay (Bimodal), and 50% Clay - 50% Pumice (Hybrid) were manufactured. As a result of the tests, it was observed that the reinforcement ceramic material was effective on the density and mechanical properties of the produced SFM. This work was financially supported by the Scientific Research Projects Department of TU Istanbul, Project No. MGA-2025-46468.

**Biography:**

Ibrahim Abdüsselam Tantoglu was born in 1997 in Istanbul. He is a thesis-stage master's student at the Istanbul Technical University, Materials and Manufacturing. He received a bachelor's degree in Manufacturing Engineering from Istanbul Technical University, Turkey. He is working at FORD OTOSAN as a Product Development Engineer. At the same time, He

is working on a master's thesis project about “Pumice and Clay Reinforced Aluminum Syntactic Foams Produced By Pressure Infiltration Technique”.

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## Day 3- Room B

### Invited Talk

#### **Ball milling and annealing effect in structural and magnetic properties of copper ferrite by ceramic synthesis**

*P. de la Presa<sup>1</sup>\*, M.A. Cobos<sup>1</sup>, J. A. Jiménez<sup>2</sup>, I. Llorente<sup>2</sup>, A. Hernando<sup>1</sup>*

*<sup>1</sup>Institute of Applied Magnetism, Complutense University of Madrid, Spain,*

*<sup>2</sup>Centro Nacional de Investigaciones Metalúrgicas (CENIM-CSIC), Avda. Gregorio del Amo, 8, Madrid 28040, Spain.*

#### **Abstract:**

This study aims to better understand the relationship between the microstructure and magnetic properties of copper ferrite, an inverse spinel that exhibits a body-centered tetragonal structure with a pronounced Jahn–Teller (JT) effect. In this study, a copper ferrite sample was synthesized via the ceramic route using a stoichiometric mixture of CuO and Fe<sub>2</sub>O<sub>3</sub> powders. These precursors were mechanically activated in a high-energy planetary ball mill and later subjected to different annealing temperatures and times in order to obtain cubic as well as tetragonal spinel structures. The samples were further subjected to severe plastic deformation through ball milling aiming to produce samples with different cationic inversions.

Interestingly, the cubic sample is unchanged by the milling and annealing processes. The observed variations in its saturation magnetization were attributed to changes in defect density. In contrast, in the tetragonal spinel, copper cations consistently occupied the octahedral sites. Milling induced a slight reduction in the inversion degree to 0.95.

This study highlights the strong correlation between structural and microstructural features—such as defects, degree of inversion, and phase composition—and the resulting magnetic properties of copper ferrite.

#### **Biography:**

Patricia de la Presa is a professor at the Complutense University of Madrid, Spain, and a renowned researcher in the field of magnetism and magnetic nanoparticles. Her research focuses on the synthesis of magnetic nanoparticles and the study of their structural and magnetic properties for various technological applications. She has authored over 100 publications (with an h-index of 28 and more than 3,000 citations), participated in numerous conferences, and led approximately 30 research projects. Additionally, she holds several contracts with private companies.

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## Invited Talk

### Enhanced superballistic transport in antidot graphene superlattices

*J. Estrada-Álvarez<sup>1</sup>, J. Salvador-Sánchez<sup>2</sup>, A. Pérez-Rodríguez<sup>2</sup>, C. Sánchez-Sánchez<sup>2</sup>, V. Clericò<sup>2</sup>, D. Vaquero<sup>2</sup>, K. Watanabe<sup>2</sup>, T. Tanigushi<sup>2</sup>, E. Diez<sup>2</sup>, F. Domínguez-Adame<sup>1</sup>, M. Amado<sup>2</sup>, E. Díaz<sup>1\*</sup>*

*<sup>1</sup>Departamento de Física de Materiales, Universidad Complutense, Madrid 28040, Spain  
<sup>2</sup>Grupo de nanotecnología, USAL-Nanolab, Universidad de Salamanca, Salamanca 37008, Spain*

*<sup>3</sup>National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan*

#### Abstract:

Viscous electron flow exhibits exotic signatures such as superballistic conduction

[1]. To observe hydrodynamics effects, a 2D device where the current flow is as inhomogeneous as possible is desirable. To this end, we build three antidot graphene superlattices with different hole diameters. We measure their electrical properties at various temperatures and under the effect of a perpendicular magnetic field to demonstrate an enhanced superballistic effect

[2]. The latter, related to a transition from a non-collective to a collective regime of transport, behaves nonmonotonically with the magnetic field. We prove that the antidot superlattice is a convenient geometry for realizing hydrodynamic flow and provide valuable explanations for the technologically relevant effects of superballistic conduction

[3]. Figure 1 - (a) Optical image and schematics of the device. (b) SEM micrograph of the antidot superlattices, where the antidot diameters are  $d = 100, 200$ , and  $300$  nm. (c) Enlarged SEM micrograph for  $d = 100$  nm antidots displaying smooth edges. (d) Simulation of the Boltzmann transport equation

[4], where streamlines are average electron trajectories.

[1] R. Krishna Kumar, et al., Nat. Phys. 13, 1182 (2017).

[2] J. Estrada-Álvarez, J. Salvador-Sánchez, A. Pérez-Rodríguez, C. Sánchez-Sánchez, V. Clericò, D. Vaquero, K. Watanabe, T. Tanigushi, E. Diez, F. Domínguez-Adame, M. Amado and E. Díaz, Phys. Rev. X 15, 011039 (2025).

[3] J. Estrada-Álvarez, E. Díaz, F. Domínguez-Adame, arxiv:2502.10265 (2025).

[4] J. Estrada-Álvarez, F. Domínguez-Adame and E. Díaz, Comm. Phys. 7, 138 (2024).

#### Biography:

I studied Physics and Mathematical Engineering and am finishing my PhD on the “Effect of the geometry on the viscous electron flow in two-dimensional materials” at the Universidad Complutense de Madrid (UCM). My expertise is simulating electrical properties in arbitrary geometries and studying the exotic signatures of electron hydrodynamics. In close collaboration with experiments, including the design of the antidot superlattices and a stay at

ETH Zürich, I look for devices with reduced dissipation and applications of electron hydrodynamics.

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## Oral Talk

### **Highly uniform resistive switching performance in conductive-bridge random access memory via two-dimensional electron gas at oxide interfaces**

*Chae Hyun Lee<sup>1\*</sup>, In Su Oh<sup>1</sup>, Ju Young Sung<sup>1</sup> and Sang Woon Lee<sup>1</sup>*

*<sup>1</sup>Department of Energy System Research and Department of Physics, Ajou University, Suwon, Gyeonggi-do 16499, Republic of Korea*

#### **Abstract:**

Resistive switching random access memory (ReRAM) is considered a promising candidate to replace conventional FLASH memory due to its fast-switching speed, high density, and compatibility with crossbar architecture. Conductive bridge RAM (CBRAM), a type of ReRAM, has attracted attention. However, it suffers from non-uniform switching characteristics during repetitive operations, which are caused by the random formation and rupture of conductive filaments.

In this work, we present highly uniform resistive switching behavior in CBRAM by introducing a two-dimensional electron gas (2DEG) at the  $\text{Al}_2\text{O}_3/\text{TiO}_2$  interface, formed via atomic layer deposition (ALD). The device structure is  $\text{Cu}/\text{Ti}/\text{Al}_2\text{O}_3/\text{TiO}_2$ , where Cu/Ti serve as the active and buffer metal electrodes, and  $\text{Al}_2\text{O}_3/\text{TiO}_2$  acts as the solid electrolyte. While 2DEG has traditionally been observed in epitaxial oxide interfaces such as  $\text{LaAlO}_3/\text{SrTiO}_3$  heterojunctions, the epitaxial growth of  $\text{LaAlO}_3$  on single-crystal  $\text{SrTiO}_3$  substrates is not suitable for memory device applications due to its high processing temperature and fabrication costs. In contrast, our work demonstrates the successful formation of 2DEG in a non-epitaxial heterostructure grown by ALD. The electrons are confined within 1–2 nm out-of-plane and move freely in-plane directions, with carrier densities reaching  $10^{13}$ – $10^{14}/\text{cm}^2$ , comparable to epitaxial-LAO/STO systems. This 2DEG-enhanced interface enables stable filament formation, leading to significantly improved uniformity in switching characteristics. The CBRAM devices exhibit excellent endurance over  $10^7$  cycles. These findings suggest that incorporating 2DEG into non-volatile memory structures can offer both performance enhancement and new device functionalities.

#### **Biography:**

Chae Hyun Lee is a Ph.D. candidate in the Department of Physics at Ajou University, under the supervision of Prof. Sang Woon Lee. She received both her B.S. and M.S. degrees in Physics from Ajou University. Her research focuses on next-generation non-volatile memory devices, with an emphasis on advanced metal thin films and interface engineering. She has

experience in thin film deposition techniques such as atomic layer deposition (ALD) and sputtering, as well as structural and electrical characterization of memory devices. Her work aims to improve device performance and reliability for future memory and data storage technologies.

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## Oral Talk

### Iron-Based MOFs and MOF Composites for Sustainable Wastewater Treatment in the Circular Economy

*Victor Ramos<sup>1\*</sup>, Konstantinos N. Pantelis<sup>2</sup>, Eleni Hadjikyprianou<sup>2</sup>, Paraschos Melidis<sup>3</sup>, Spyridon Ntougias<sup>3</sup>, Anastasios J. Tasiopoulos<sup>2</sup>, Sophia A. Tsipas<sup>1</sup>*

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#### Abstract:

One of the main challenges in modern industrial society is the treatment of wastewater from industrial, agricultural, and domestic sources in a way that supports the circular economy through resource recovery and water reuse. These wastewaters often contain harmful inorganic and organic pollutants. While many purification techniques exist-such as membrane filtration, centrifugation, and reverse osmosis-adsorption is considered the most accessible due to its effectiveness, low cost, and versatility.

Although activated carbon was initially used, more economical alternatives have since been explored. Metal-Organic Frameworks (MOFs) have emerged as promising adsorbents thanks to their high porosity, tunable structures, and ease of functionalization. However, their limited stability in water-mainly due to hydrolysis-remains a drawback. Despite this, certain MOFs like MIL-100, MIL-101, UIO-66, and ZIF-8 demonstrate water stability and potential for use in wastewater treatment.

To enhance performance, MOFs can be combined with other materials such as biochars, clays, or alginate to form MOF composites (MOFCs). These composites improve stability and adsorption capacity and can be shaped into beads for easier handling. A series of MOFs and their composites-including MIL-100, MIL-101, and MIL-88A with biochar, clay, and alginate-were synthesized and characterized using PXRD, porosimetry, and thermal analysis. Their ability to adsorb organic pollutants was evaluated using UV-Vis spectroscopy, highlighting their potential in water treatment and other applications such as sustainable fertilizers.

#### Biography:

Victor Ramos is a Chemistry graduate from the University of Seville. He continued his studies at the same university with a Master's in Science and Technology of New Materials.

After a brief period at the CSIC in Seville where he worked with MOFs for biomedical purposes, he is currently pursuing a PhD in the framework of the "CIRQUA" Project, part of the PRIMA programme, supported by the European Union (Grant agreement No. 2321 call 2023 Section 1), focused on the water treatment and fertilization of soils.

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## Oral Talk

### Ultrafast hydrogen sensing technology based on nanoscale metal filaments

*In Su Oh<sup>1\*</sup>, Chea Hyun Lee<sup>1</sup>, Sang Woon Lee<sup>1</sup>*

*<sup>1</sup>Ajou University, Republic of Korea*

#### Abstract:

Hydrogen is a promising clean energy source. However, its high flammability and colorless, odorless nature necessitate the development of rapid and highly reliable detection technologies. Now, the hydrogen detection time has been at least a few seconds. In this study, we propose an ultrafast hydrogen sensor based on a novel hydrogen sensing mechanism via the formation and rupture of nanoscale metal filaments within a conductive-bridge random access memory (CBRAM) device. A two-dimensional electron gas (2DEG) formed at oxide heterointerfaces was used as the bottom electrode to achieve precise filament control and stable repetitive operations.

In the hydrogen sensor, nanoscale metal filaments are formed by electrical writing and ruptured upon hydrogen exposure. The hydrogen introduces extra heat to the metal filaments, which then rupture due to the Joule heating process. The accumulated thermal energy destabilizes the filament, promoting its rupture and leading a rapid increase in sensor resistance. The proposed mechanism offers significantly faster response times than the microsecond scale, compared to conventional hydrogen sensors based on chemical reactions or gas diffusion. In addition, it leverages the advantages of CBRAM, including compatibility with semiconductor fabrication processes, low power consumption, and high scalability, enabling not only the development of practical sensing platforms but also application to crossbar array architectures for enhanced detection accuracy across a wide range of hydrogen concentrations. Experimental validation confirms that hydrogen-induced thermal environmental changes can be directly transduced into electrical signals, enabling ultrafast hydrogen sensing. This study proposes a new sensing paradigm for ultrafast and highly reliable hydrogen detection.

#### Biography:

In Su Oh is a Master's student in the Department of Physics and the Department of Energy Systems Research at Ajou University, where he also earned his bachelor's degree in Physics. His research focuses on nanoscale memory devices, particularly Conductive-Bridge Random Access Memory (CBRAM), and the formation of two-dimensional electron gas (2DEG) structures by atomic layer deposition (ALD). He is currently investigating ultrafast hydrogen



sensing mechanisms based on filament dynamics in CBRAM structures. His broader research focuses on developing novel materials and device architectures for next-generation semiconductor devices.

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## Oral Talk

### High-Performance Thin-Film Transistors Enabled by Two-Dimensional Electron Gas at Oxide Heterostructures

*Sang Hyeok Lee\*, Ju Young Sung, Chae Hyun Lee, Yebin Lim, In Su Oh, Kyoung Hyeon Choi, Sang Woon Lee*

*Department of Physics, and department of Energy Systems Research, Ajou University, Republic of Korea*

#### Abstract:

Two-dimensional electron gas (2DEG) was observed at the epitaxial interface of oxide heterostructures such as LaAlO<sub>3</sub>/SrTiO<sub>3</sub>. 2DEG formation at the epitaxial LAO/single-crystal STO interface is attributed mostly to ‘polar catastrophe’, which explains the accumulation of electrons at the interface to avoid a potential divergence across the LAO/STO heterostructure. Unfortunately, fabrications of epitaxial layer using single crystalline substrates are unsuitable for practical applications due to the high cost of producing oxide single crystal and epitaxial layer.

Recently, we reported that 2DEG can be formed at the non-epitaxial Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> interface using atomic layer deposition (ALD). 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. The 2DEG density approaches  $\sim 10^{14}$  cm<sup>-2</sup> and it can be tuned between  $10^{13}$ ~ $10^{14}$ /cm<sup>2</sup> by adjusting the ALD process temperature of the Al<sub>2</sub>O<sub>3</sub> layer. We demonstrate high-performance thin-film transistors using this semi-metallic 2DEG as the channel, exhibiting high transconductance, excellent spatial uniformity, and effective gate control over the drain current. The ultrathin TiO<sub>2</sub> bottom layer is easy to fully deplete, allowing an extremely low off-current, a high on/off-current ratio over 10<sup>8</sup> and a low sub-threshold swing of  $\sim 100$  mV/dec. By implementing ALD, a mature thin film process can facilitate mass production as well as three-dimensional integration of the devices. Considering that the ALD process is a technically-mature process in the present semiconductor field, this work will enable the mass-production of 2DEG devices and allow complicated multi-level device integrations such as gate-all-around and multi-gated transistors and 3D-stacked FETs.

#### Biography:

I am currently pursuing a Master of Science (M.S.) degree in the research group of Professor Sang Woon Lee at Ajou University. My research focus on thin film deposition using Atomic Layer Deposition(ALD), and manufacture nano transistor device. I am investigating high-performance transistor devices based on semimetallic 2DEG layers, with an emphasis on

gate-controlled transport and scalable device architectures. My broader interests include quantum transport phenomena, and the development of next-generation oxide-based nanoelectronic systems.

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### **Oral Talk:**

## **Exploration of Alternative ALD Reactions to Reduce the Resistivity of TiN Thin Films for DRAM Capacitor Electrodes**

*Byeong Jun Jeon<sup>1\*</sup>, Kyeong Hyeon Choi<sup>1</sup>, Se Eun Kim<sup>1</sup>, Kyung Joon Lee<sup>1</sup> and Sang Woon Lee<sup>1</sup>*

*<sup>1</sup>Department of Physics / Department of Energy Systems Research, Ajou University, Republic of Korea*

### **Abstract :**

Transition metal nitride thin films, such as Titanium nitride (TiN), are widely used as electrode materials in dynamic random access memory (DRAM) devices due to their excellent electrical conductivity. However, conventional TiN atomic layer deposition (ALD) processes using Ti-chloride precursors and ammonia (NH<sub>3</sub>) often result in a high amount of residual chlorine impurity (>3%) within the TiN films at deposition temperatures around 400°C. These chlorine residues, originating from the strong Ti–Cl chemical bonds in the precursor, lead to increased film resistivity.

In this study, an alternative ALD surface reaction pathway is proposed to reduce chlorine impurity concentration by introducing an additional hydrogen sulfide (H<sub>2</sub>S) gas pulse between the Ti-chloride and NH<sub>3</sub> pulse steps. The H<sub>2</sub>S reacts with the Ti precursor to form a titanium sulfide (TiS<sub>x</sub>) intermediate with a weaker bonding energy than original Ti-Cl bond, thereby enabling more efficient ligand exchange with NH<sub>3</sub> and resulting in the deposition of high purity TiN films with reduced chlorine impurities.

Compared to the conventional process, the alternative ALD scheme achieved over a 50% reduction in residual chlorine concentration at 400°C and led to more than a 20% decrease in film resistivity. These results demonstrate the effectiveness of the H<sub>2</sub>S-assisted ALD approach in improving the material quality and electrical property of TiN thin films. This alternative ALD process is a practical solution for achieving high-quality TiN integration in advanced DRAM technologies.

### **Biography:**

Byeong Jun Jeon is currently pursuing his M.S. degree in the Department of Physics at Ajou University, Republic of Korea, under the supervision of Prof. Sang Woon Lee. Where his

research focuses on the atomic layer deposition (ALD) of next-generation electrode and dielectric thin films for DRAM capacitors. His research interests include thin film deposition process development and electrical property characterization for advanced semiconductor applications.

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## Oral Talk

### **Automotive textile thermal resistance enhancement for high temperature functionalization**

*José Abreu<sup>1\*</sup>, Neslihan Akcay<sup>2</sup>, João Rodrigues<sup>2</sup>, Pedro Anacleto<sup>2</sup>, João Juliana P.S. Sousa<sup>2</sup>, José Gouveia<sup>3</sup>, Inês Alves<sup>3</sup>, Jorge Padrao<sup>1</sup>, Ana Maria Rocha<sup>1</sup>*

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#### **Abstract:**

Textiles commonly used by the automotive industry display relevant thermal robustness for the temperatures experienced inside a cabin environment and the common functionalization processes. However, advanced functionalization methods, such as chemical vapor deposition, may demand higher thermal resistance from textiles over prolonged periods. Improving the thermal resistance of common textile materials, such as polyester (PES), to withstand such conditions without compromising structural integrity and mechanical performance remains a considerable challenge<sup>1</sup>. The applicability of vermiculite and silica oxide was explored to enhance the thermal properties of PES woven sunscreen typically used in car sunroofs (AA4088, COPO Textile)<sup>2,3</sup>. Vermiculite's suitability stems from its distinctive two-dimensional layered structure, which imparts excellent thermal stability and expansion capacity<sup>4,5</sup>. In addition, silica oxide exhibits a remarkable thermal and corrosive stability, key features for the proposed application<sup>6</sup>. To enable photovoltaic functionalization via chemical vapor deposition at elevated temperatures, two different methods and their combination were evaluated for their efficiency and industrial scalability potential. The use of vermiculite dispersion (DM677, Dupré Minerals) through padding and/or knife coating, and sol-gel for functionalization through exhaustion method. The sol-gel processes allowed the silica oxide based nanocoating of PES. Characterization of the different application configurations included microscopy, thermogravimetric analysis (TGA), attrition coefficient, and profilometry. Furthermore, mechanical characterization was performed to ensure adequate flexibility of the functionalized PES. Finally, functionalized PES samples subjected to 300 and 500 °C for 1 hour exhibited an impressive thermal resistance.

**Biography:**

José Abreu holds a Master's Science degree in Textile Engineering from the University of Minho, with a specialization in Advanced Materials and Technologies, and has received several academic distinctions throughout his academic path. He is currently conducting research at the Centre for Textile Science and Technology (2C2T) within the scope of the Green Auto project, focused on the development of advanced materials and coatings for the automotive sector. He is the author and co-author of scientific publications submitted to indexed international journals and has participated in scientific events in the field of smart and e-textiles.

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