MATERIALS Europe

PRISM

3rd INTERNATIONAL CONGRESS ON

MATERIALS SCIENCE AND ENGINEERING

JULY 15–17, 2026 | POLITECNICO DI MILANO
PIAZZA LEONARDO DA VINCI, MILAN, ITALY

ABSTARCT BOOK

HOSTING UNIVERSITY

POLITECNICO MILANO 1863

SPONSOR

FAVS Scientific Equipment di Gnudi Andrea e Antonella S.r.l.

EXHIBITORS

frontiers in Batteries and Electrochemistry

frontiers in Carbon

www.materialsconferenceeurope.com

MATERIALS EUROPE 2026

ABSTRACT BOOK

DAY – 1

PLENARY SESSION

Membrane-Targeted Azobenzenes: New Interfaces Between Light and Biological Systems

Chiara Bertarelli, Politecnico Milano, Italy

Abstract:
The development of molecular systems capable of bridging optical stimuli and biological responses is opening new opportunities at the interface between materials science and life sciences. Among these, membrane-targeted azobenzenes represent a unique class of photoresponsive materials that operate directly within biological membranes, where light-induced isomerisation can be transduced into functional cellular responses.

In this lecture, I will discuss the design principles underlying amphiphilic azobenzenes and their interaction with biological membranes, focusing on Ziapin2 and push-pull systems as a versatile molecular platform. The ability of these photoswitches to couple ultrafast photoisomerisation with membrane mechanical and electrical properties has enabled non-genetic optical modulation in a variety of biological systems, ranging from excitable mammalian cells to microbial systems.

Recent developments extending this concept beyond the plasma membrane will also be presented. These advances illustrate how molecularly engineered azobenzenes can provide new tools for studying and controlling complex biological functions, establishing novel connections between materials design, photophysics, and living systems.

Biography:

Prof. Chiara Bertarelli is Full Professor of Materials Science and Technology at Politecnico di Milano. She received her PhD in Materials Engineering from Politecnico di Milano and has held visiting positions at Shinshu University in Japan and École Normale Supérieure de Cachan in France.

Her research focuses on functional organic and hybrid materials, including photoresponsive materials, organic semiconductors, nanofibers, and biointerfaces. She is particularly known for the development of membrane-targeted azobenzenes, a class of light-responsive materials that create new interfaces between light and biological systems.

She has authored 170 peer-reviewed publications and is co-inventor of five patents.

Shaping Tomorrow's Electronics: Alternatives to Silicon

***Rodrigo Martins**, P. Barquinha, L. Pereira, R. Silva, D. Vieira, E. Carlos, A. Kiazadeh, J. Pinto, S. Nandy, D. Gaspar, E. Fortunato*
CENIMAT|i3N, Department of Materials Science, School of Science and Technology, NOVA University Lisbon and CEMOP/UNINOVA, Caparica, Portugal

Abstract
In the digital age, rapid technological advancements present critical sustainability challenges, including material scarcity, increasing waste, and environmental pollution, often aggravated by high-temperature manufacturing processes. The socio-economic growth fueled by the demand for smart electronics and non-recyclable materials further exacerbates climate change and resource depletion.

As we embrace the Internet of Things (IoT) and wearable technology, the urgency for sustainable materials intensifies. Emerging nanoscale devices offer promising alternatives to traditional silicon-based options, particularly in the realm of transparent and paper electronics, which hold the potential to revolutionise our approach to electronic devices.

This presentation delves into strategies for minimising electronic waste while advancing eco-friendly technology solutions. We are dedicated to developing green electronic products that fulfil consumer needs and promote environmental stewardship, transitioning from micro- to nanoscale innovations. Our initiatives also focus on raising social awareness about sustainable technologies, actively engaging with communities and policymakers to advocate for practices that align technology with environmental responsibility.

Join us on this journey to explore innovative approaches to sustainability, as we aim to create a meaningful impact on our environment and cultivate a resilient future empowered by green technology.

Biography:

Rodrigo Martins, full professor at FCT-NOVA, expert in Advanced Functional Materials for electronics and energy applications, with more than 1375 papers published, cited more than 44,500, with an h-index of 105. Running president of the European Academy of Sciences, director of the Associated Laboratory i3N, the Institute of Nanostructures, Nanomodeling and Nanofabrication; President of the administration board of the Portuguese cluster in Advanced Materials (NANOMAT); member of the administration board of the Portuguese cluster on Batteries (BatPower); chair of the European committee affairs of European Materials Research Society; editor in chief of the journal Discover Materials. Coordinator of Emerging Printed Electronics Research Infrastructure (EMERGE), the first in Europe beyond Silicon.

He is a member of: Academia Europaea; Royal Academy of Sciences and Arts of Barcelona; Portuguese Academy of Engineering; the Portuguese Order of Engineers; advisory board (2025-2027); European University for Customised Education (EUNICE),; editorial board of the journal Innovation Material (2025-2027). Co-chair of the FNRS (Fonds de la Recherche Scientifique, Belgium) Quinquennial Scientific Prize, A DE LEEUW-DAMRY-BOURLART Prize in Applied Exact Sciences. QiuShi Chair Visiting Professor at Zhejiang University; Honorary Professor of Hefei Institutes of Physical Sciences of the Chinese Academy of Sciences (CAS); Honorary Professor of the Technical University of Wuhan and of the School of Chemistry, Chemical Engineering and Life Sciences of Wuhan University; Honorary Professor of Fuzhou University; invited Professor at Southwest University, Chongqing, China. In 2023, selected as a PIFI Distinguished Scientist of China and honoured in 2025 with the Chinese Government Friendship Award.

Former: President of the International Union of Materials Research Societies (IUMRS); member of the Scientific Council of the European Research Council; Advisory Council of DG Prosperity, European Programme Horizon.

Nanocomposite Polymeric Membranes for H_2 Separation and CO_2 Capture

(Neal) Tai-Shung Chung

[1]Graduate Institute of Applied Science and Technology, Department of Chemical Engineering, Department of Materials Science and Engineering, National Taiwan University of Science and Technology (NTUST).

[2]Emeritus Professor, National University of Singapore (NUS)

Abstract:

Clean water, clean energy, global warming and affordable healthcare are four major concerns globally resulting from clean water shortages, high fluctuations of oil prices, climate change and high costs of healthcare. Clean water and public health are also highly related, while clean energy is essential for sustainable prosperity. Among many potential solutions, advances in membrane technology are one of the most direct, effective and feasible approaches to solve these sophisticated issues. Membrane technology is a fully integrated science and engineering that consists of materials science and engineering, chemistry and chemical engineering, separation and purification phenomena, environmental science and sustainability, statistical mechanics-based molecular simulation, and process and product design. In this presentation, we will introduce our efforts on membrane R&D for H_2 purification and separation, and CO_2 capture from flue gas. Various material and fabrication strategies of both dense-flat and hollow fibre membranes to enhance membrane performance will be discussed.

Biography:

Prof. Chung is a Jade Mountain Chair professor at NTUST, Taiwan. Before joining NTUST, he was a Provost's Chair Professor at the ChBE dept of the National University of Singapore from 2011 to 2021. His research focuses on polymeric membranes for clean water, clear energy and pharmaceutical separation. He became a Fellow in the Academy of Engineering Singapore in 2012. He received the Underwood Medal from IChemE (Institute of Chemical Engineers, UK) for exceptional research in separations and the Singapore President's Technology Award in 2015. He was ranked as No. 7th in Chemical Engineering worldwide by "the top 2% scientists in the world" published by Stanford University in 2025. His H-index ≥ 142 (Scopus) or 164 (Google Scholar). His recent world rankings by https://research.com/u/tai-shung-chung in the fields of Chemistry and Materials Science in 2025 are as follows:

	D-index	Citations	World ranking	Taiwan Ranking
Chemistry	**158**	**82,340**	**83**	**1**
Materials Science	**153**	**79,121**	**116**	**1**

Benign-by-design nanomaterials for catalysis and energy-related applications

Rafael Luque

People's Friendship University of Russia (RUDN University), 6 Miklukho Maklaya Str., 117198, Moscow, Russian Federation

Universidad ECOTEC, Km. 13.5 Samborondón, Samborondón, EC092302, Ecuador

Abstract

The development of benign-by-design nanomaterials is opening new opportunities for sustainable catalysis and energy-related applications. This presentation highlights recent advances in the design and synthesis of environmentally friendly nanostructured materials, with particular emphasis on mechanochemical approaches, metal–organic frameworks (MOFs), and tailored nanostructures for catalytic and electrochemical processes. Their applications in energy storage, photocatalysis, biomass valorisation, and environmental remediation are discussed, together with innovative strategies for catalyst stability under continuous-flow conditions and the recycling of waste-derived catalytic materials. These examples demonstrate how green chemistry principles can be integrated with advanced

materials design to produce highly active, stable, and sustainable systems for future energy and environmental technologies.

Biography:

Rafael Luque (PhD in 2005 from Universidad de Cordoba, Spain) has significant experience in biomass and waste valorisation practices to materials, fuels and chemicals, including nanoscale chemistry, green chemistry and catalysis, as well as environmental remediation with a particular interest in plastic waste (>1000 publications, h-index 125, >70,000 citations, 7 patents, >10 edited books). He was named a 2018-2022 Highly Cited Researcher (Clarivate Analytics) and received Honorary Professor titles (Doctor Honoris Causa) at Universitá degli Studi Mediterranea di Reggio Calabria and RUDN University.

Prof. Luque is currently Head of B4 group (Bioresources, Biopolymers, Biotechnology and Biorefineries) and Project Director at National University of Science and Technology Polytehnica Bucharest (Romania), holding various positions as DFSP Chair Professor at King Saud University (Saudi Arabia), Distinguished Visiting Professor at University of Lahore (Pakistan), Adjunct Professor at Chulalongkorn University (Thailand) and International Distinguished Scientist and Rectoral Advisor at Universidad ECOTEC (Ecuador).

Session: Innovations in Materials Synthesis and Characterisation

Keynote Talk

NMR Spectroscopy for Materials Science and Pharmaceuticals

Franca Castiglione

Department of Chemistry, Materials and Chemical Engineering "Giulio Natta", Politecnico di Milano, Milan, Italy

Abstract

Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful and versatile analytical technique for probing the structure, dynamics, and molecular organisation of complex systems across materials science and pharmaceutical research. In materials science, advanced solid-state and solution NMR methods provide atomic-level information on polymers, biomaterials, nanostructured systems and functional materials, enabling the characterisation of local environments, molecular mobility and intermolecular interactions that are often inaccessible by other analytical techniques. Particular attention has recently been devoted to ionic liquids (ILs) and deep eutectic solvents (DESs), whose unique physicochemical properties make them promising materials for sustainable technologies. NMR spectroscopy plays a crucial role in elucidating the molecular structure, ion pairing, hydrogen-bonding networks, and transport properties of these systems. In the field of energy storage, multinuclear and diffusion NMR techniques provide fundamental insights into ion dynamics and electrolyte behaviour, supporting the development of advanced electrolytes for next-generation batteries.

In pharmaceutical sciences, NMR spectroscopy is extensively employed for the characterisation of active pharmaceutical ingredients (APIs), polymorphism and drug–polymer interactions. Moreover, DESs are emerging as innovative media for drug solubilization-delivery, and NMR 2D methods are used to investigate their supramolecular organisation and interactions with pharmaceutical compounds. The continuous advances in high-field instrumentation and solid-state magic-angle spinning (MAS) and multidimensional experiments have considerably expanded the capabilities of NMR spectroscopy. By bridging materials science, energy research, and pharmaceutical technology, modern NMR provides an indispensable platform for understanding structure–property relationships and guiding the rational design of advanced functional materials and drug delivery systems.

Keynote Talk

Liquid Interface Deposition (LID) : A method for the production of thin films and heterostructures of two-dimensional solids

Marek Szablewski, A.R. Smith, and M.R.C. Hunt

Dept. of Physics, Durham University, South Road, Durham DH1 3LE, U.K

ABSTRACT:

A novel technique – 'Liquid Interface Deposition' (LID) – for the production of ultra-thin films and heterostructures of two-dimensional solids is presented. The method is applicable to any two-dimensional material derived from, or equivalent to, a bulk layered solid with van der Waals interlayer bonding and enables controlled deposition onto any substrate of arbitrary shape without the requirement for prior surface treatment.

We describe the LID technique, the science that underpins it and give examples of the two-dimensional materials which have been successfully deposited using it, including graphene and molybdenum disulfide, amongst others. Physical and chemical characterisation of structures built using the LID technique is reported, as well as a discussion of their possible applications.

Keynote Talk

Gas-Phase Synthesis of Hybrid Nanoparticles Driven by Magnetron Sputtering

Andrei Choukourov1, Daniil Nikitin1, Iqra Wahid1, Ronaldo Katuta1, Veronika Červenková1, Hynek Biederman1*

1Charles University, Faculty of Mathematics and Physics, Department of Macromolecular Physics, Czech Republic

Abstract:

Sputter-driven gas aggregation is a well-established and highly versatile technique for the synthesis of metal nanoparticles (NPs). In this approach, atomic metal vapor generated by magnetron sputtering condenses in a cold inert gas atmosphere, enabling the formation of nanoparticles with controllable size and composition. Traditionally, planar magnetrons have been employed as sputtering sources; however, the progressive evolution of their erosion tracks limits long-term process stability, reproducibility, and precise control over NP production. Cylindrical magnetrons provide an effective solution to these limitations by offering a uniform erosion profile and significantly extended target lifetime. Despite their widespread application in thin-film deposition, cylindrical magnetrons have so far not been systematically explored for gas-phase nanoparticle synthesis. In this contribution, we

demonstrate and compare the use of dc planar and cylindrical magnetrons for the gas-phase production of metal nanoparticles. The approach enables the synthesis of monometallic as well as hybrid bimetallic nanoparticles exhibiting complex morphologies, including core@shell and Janus-type structures. Furthermore, we present reactive sputtering experiments conducted in Ar/N_2 gas mixtures, allowing the formation of metal nitride (MeN) nanoparticles, where Me = Ti, Zr, Hf, Cu, or Fe. By systematically varying the gas composition, working pressure, and discharge current, we achieve precise control over nanoparticle size distributions and chemical composition. The synthesised nanoparticles exhibit strong potential for applications in refractory plasmonics, solar-light harvesting, and electrochemical CO_2 reduction. Representative experimental results and structure–property relationships will be discussed.

Acknowledgments

The work was supported by the Czech Science Foundation via grant GACR24-11398S.

Keynote Talk

Intercalation Phase Engineering of Transition Metal Dichalcogenides

*Zhiyuan Zeng1**

1 Department of Materials Science and Engineering, and State Key Laboratory of Marine Environment Health, City University of Hong Kong, Hong Kong 999077, P. R. China

Abstract:

Intercalation of atoms, ions, and molecules is an effective means of tuning the properties of two-dimensional materials, while in situ imaging and spectroscopy provide powerful tools for deciphering intercalation dynamics and mechanisms.1,2 Firstly, we developed a lithium ion battery intercalation & exfoliation method with detailed experimental procedures for the mass production of 11 2D transition metal dichalcogenides (TMDs) and inorganic nanosheets, such as MoS2, WS2, TiS2, TaS2, ZrS2, graphene, h-BN, NbSe2, WSe2, Sb2Se3 and Bi2Te3, among them 3 TMDs achieved mono- or double layer yield > 90%.3 The Li insertion can be monitored and finely controlled in the battery testing system, so that the galvanostatic discharge process is stopped at a proper Li content to avoid decomposition of the intercalated compounds. Secondly, we discovered that small current and high cut-off voltage (0.005 A g-1, 0.9 V) produces pure 2H WS2 bilayers. while large current and low cut-off voltage (0.02 A g-1, 0.7 V) leads to 1T' WS2 monolayers.4 For the lithium intercalation mechanism, state-of-the-art in-situ liquid phase transmission electron microscopy (TEM) is an ideal technique for identifying phase changes in TMDs during the lithium intercalation process.5,6 When combined with in-situ X-ray absorption spectroscopy (XAS), X-ray diffraction (XRD), and Raman spectroscopy, the underlying mechanisms of intercalation phase engineering can be elucidated, enabling the phase-switchable preparation of TMDs.7 Regarding application,

the unconventional (metastable) TMDs phases generated and stabilized via intercalation demonstrate significantly enhanced physical and chemical properties for a variety of applications, such as superconducting quantum devices, thermoelectric generator,7 humidity sensor,4 heavy metal removal,8 ion separation,9-12 and environmental DNA detection,13 among others.

References:

[1] R. Yang†, L. Mei†, Z. Lin†, et al., Q. Lu*, J. Li*, Z. Y. Zeng*, Nat. Rev. Chem., 2024, 8, 410.

[2] R. Yang, et al., D. Voiry, Q. Lu, J. Li*, Z. Y. Zeng*, Nat. Synth., 2023, 2, 101-118.

[3] R. Yang, L. Mei, et al., H. S. Shin*, D. Voiry*, Z.Y. Zeng*, Nat. Protoc., 2022, 17, 358-377.

[4] L. Mei, Z. Gao, R. Yang, et al., J. Li*, X. Yu*, Z. Y. Zeng*, Nat. Synth., 2025, 4, 303-313.

[5] R. Yang, L. Mei, Y. Fan, et al., J. Yang, J. Li*, Z. Y. Zeng*, Nat. Protoc., 2023, 18, 555-578.

[6] Q. Zhang†, J. Ma†, L. Mei, J. Liu, Z. Li*, J. Li*, Z. Y. Zeng*, Matter, 2022, 5, 1235-1250.

[7] Q. Zhang, et al. K. Loh*, Z. Zeng*, Natl. Sci. Rev., 2026, 2026, DOI: 10.1093/nsr/nwag165.

[8] L. Mei, M. Sun, et al., B. Huang*, L. Gu*, D. Voiry, Z. Y. Zeng*, Nat. Commun., 2024, 15, 7770.

[9] T. Ying, N. Onofrio, et al., C. Y. Tang*, D. Voiry*, Z. Y. Zeng*, Adv. Mater., 2025, 37, e04781.

[10] T. Ying, Y. Xiong, et al., C. Y. Tang, J. Fan, Z. Y. Zeng*, Adv. Mater., 2024, 36, 2403385.

[11] L. Mei, et al., D. Voiry, H. Wang*, A. B. Farimani*, Z. Y. Zeng*, Adv. Mater., 2022, 34, 2201416.

[12] Y. Zhang, et al., B. Huang*, Z. Y. Zeng*, Nano Lett., 2026, DOI: 10.1021/acs.nanolett.5c04248.

[13] L. Mei, et al., Z. Y. Zeng*, K. M. Y. Leung*, Natl. Sci. Rev., 2026, DOI: 10.1093/nsr/nwag055.

INVITED TALK

Plasma Polymerisation of Hydrocarbon Precursors for the Synthesis of Nanofuels for Proton-Boron Fusion

Daniil Nikitin1, Marco Tosca1,2, Kateryna Biliak1, Mariia Protsak1, Jan Hanuš1, Veronika Červenková1, Ronaldo Katuta1, Jakub Čížek1, Daniel Molloy3, Marco Borghesi3, Eric Hirschmann4, Jaakko Julin5, Lorenzo Giuffrida2, Daniele Margarone2, Andrei Choukourov1

1Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

2ELI Beamlines Facility, the Extreme Light Infrastructure ERIC, Dolni Brezany, Czech Republic

3Centre for Light-Matter Interactions, School of Maths and Physics, Queen's University Belfast, UK

4Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany

5University of Jyväskylä, Department of Physics, Jyväskylä, Finland

Abstract:

Materials containing hydrogen and boron are promising candidates for laser-driven proton–boron (pB) fusion, a reaction that produces energetic α-particles without neutron emission or radioactive waste. In this approach, an ultrashort, high-intensity laser pulse irradiates a solid target, ionising the material and accelerating protons to energies sufficient for fusion with boron nuclei. The generated α-particles could be used in applications such as sustainable energy production, space propulsion, radiobiology, and cancer therapy. Most experimental demonstrations of laser-driven pB fusion have relied on macroscopic targets composed of boron-containing materials, such as boron nitride, combined with hydrogen-rich polymers. However, their efficiency is limited by poor laser energy absorption by the target surface, thereby restricting proton acceleration and reducing the α-particle yield. Nanostructured and porous fuels may overcome this limitation because sub-micrometre features enhance laser absorption and plasma formation. In this work, we developed nanostructured fusion fuels based on plasma-polymerised hydrocarbon nanoparticles (NPs) produced in a gas aggregation source. Hexane, cyclohexane, and benzene precursors were polymerised under different radio-frequency discharge powers, forming micrometre-thick coatings composed of porous NP assemblies. The NP diameters in all the cases were above 100 nm. Positron annihilation lifetime spectroscopy revealed a hierarchical pore structure consisting of sub-nanometer free volumes within the plasma polymer and larger interparticle voids. Elastic recoil detection analysis showed that about 50% of the hydrogen from precursor molecules was retained, with hexane-derived NPs exhibiting the highest content. Targets prepared from these NPs successfully initiated pB fusion when irradiated by the TARANIS laser (10 J, 800 fs, 2 × 1019 W/cm2), producing α-particles fluxes comparable to the highest reported values.

INVITED TALK

Influence of Ag content of Polyethene Glycol/Silver (PEG/Ag) Nanocomposite Thin Films on AC Conductivity

Sahin Yakut1, Maria Naz2, Huseyin Furkan Eminoglu1, Deniz Bozoglu1, Deniz Deger1, Kemal Ulutas1

1Istanbul University, Faculty of Sciences, Department of Physics, Turkey

2Istanbul University, Institute of Graduate Studies in Sciences, Turkey

Abstract:

Polyethene glycol (PEG) nanocomposites with silver (Ag) content ratios of 10%, 20%, 30%, and 40% were prepared via thermal evaporation of PEG and e-beam evaporation of Ag. The resultant PEG/Ag nanocomposites were investigated using dielectric spectroscopy measurements. The presence of Ag in polymers is known as an antibacterial agent. In this study, we aimed to detect the effect of Ag content in the nanocomposite structure in the aspect of electrical conduction by checking the DC-like region of AC conductivity behaviour, which can be observed at the lowest frequency side of radio frequency (RF) dielectric spectroscopy spectra. This study also aims to investigate the conduction mechanisms and the effect of Ag content on the barrier width between localised sites in polycrystalline or amorphous structures of PEG/AG nanocomposite thin films.

For a PEG thin film that does not include Ag atoms, the DC-like conductivity is between 10-12 and 10-11 S/cm, with an increasing trend with temperature. Moreover, three conduction mechanisms were observed in the investigated frequency interval. These may be the drift motion of partially free charge groups (fragments) produced by polymer chain fragmentation by thermal evaporation at low frequencies and high temperatures. Another mechanism may be the orientational polarisation of oligomers, which is produced by the breaking of the polymer main chain by shifting at lower temperatures and higher frequencies by thermal evaporation. The last mechanism is observed by shifting at the highest frequencies and at nearly all temperatures. When the effect of Ag content is investigated, the DC-like region shifts toward 10-10-10-9 S/cm interval with almost ten times increase for the %40 Ag-containing PEG/Ag thin film. The mid-frequency region vanishes or becomes difficult to detect for Ag-containing thin films. These results may be attributed to the joining of some Ag atoms to semi-free charge groups. Additionally, some Ag atoms may be bonded to oligomers by shifting the polarisation frequencies toward lower frequencies in the investigated frequency region. Moreover, this shifting may be

The reason for the increase in DC-like conductivity values is the coincidence of the polarisation regions of drifting semi-free charge groups and orientationally polarized high-weighted oligomers.

INVITED TALK

EFFECT OF PRIMARY CARBIDES ON THE FATIGUE BEHAVIOR OF AIRCRAFT TURBINE BEARING STEELS

*Víctor M. Alcántara Alza,**

Department of Mechanics and Energy-- Trujillo National University-Perú

Abstract

The fatigue performance of all high-strength steels is affected by internal defects. Primary carbides have been shown to be the main type of defects in M50 bearing steels used in the aerospace industry. Therefore, these steels must be characterised under service conditions, and their rolling contact fatigue (RCF) properties must be evaluated under different friction conditions. A method for analysing the response of primary carbides is proposed;

Furthermore, the RCF process is separated into a period of plastic instability and an elastic period. The accumulation of plastic deformation around the carbides before elastic deformation is proposed as the RCF damage parameter, and the influence of primary carbides is studied based on the damage criterion. The competition between surface and internal fatigue initiation is revealed through different coefficients of friction. A predictive model for RCF initiation is proposed, which could predict critical sizes for different types of primary carbides that are not detrimental to RCF performance, and critical sizes are calculated under typical industrial service conditions

Keywords: fatigue in steels; M50 Bearing steels; Rolling Contac fatigue; primary carbides

Room – B

Session: Computational Design, Synthesis and Characterisation of Advanced Materials

Keynote Talk

New structural properties and host-guest chemistry of M12L8 polycatenanes

Javier Martí-Rujas, Politecnico di Milano, Chemistry, Materials and Chemical Engineering "Giulio Natta" Milano, Italy

Abstract:

Poly-[n]-catenanes (PCs) formed of interlocked metal organic cages (MOCs) self-assembled of 12 metals (M) and 8 ligands (L) (hereafter PCs-MOCs)1 are a new class of emerging functional materials combining the properties of mechanically interlocked materials (MIMs),2 the internal space of MOCs, and the structural features of polymers. PCs-MOCs are currently studied not only for their aesthetic aspects, but also for their potential applications in gas adsorption, electron conductivity and X-ray attenuation.1 Despite the recent progress in the field, there are many structural aspects that need to be understood to fully exploit PCs-MOCs as functional materials.

In this lecture, the latest results in the host-guest chemistry of PCs-MOCs self-assembled using the symmetric exotridentate tris-pyridyl benzene (TPB) ligand and ZnX2 (where X= Cl, Br, I), Figure 1, will be presented. The polymeric structure (1) is composed of interlocked M12L8 icosahedral nanometric cages with internal voids of ca. 2700 Å3.3 The interlocked nanocages can be synthesised very fast, homogeneously, and in large amounts as microcrystals under kinetic control. Slow crystallisation also yields large single crystals amenable to crystal-to-crystal guest exchange processes that have been used to study molecular recognition of aromatics via gas-solid reactions.4 The high density of mechanical bonds in 1 enhances the structural stability and gives a dynamic response upon external stimuli. Such mechanical and structural properties can be used to exploit the host-guest chemistry of the large voids present in the M12L8 nanocages of 1.

Figure 1. Synthesis of the M12L8 interlocked nanocages forming the poly-[n]-catenane 1 and some of its key structural features was studied.

References.

[1] J. Martí-Rujas and A. Famulari, Angew. Chem. Int. Ed. 2024, 63, e202407626.

[2] J. F. Stoddart, Chem. Soc. Rev., 2009, 38, 1802

[3] S. Torresi, A. Famulari and J. Martí-Rujas, J. Am. Chem. Soc., 2020, 142, 9537-9543.

[4] J. Martí-Rujas, S. Elli, A. Zanotti, A. Famulari and F. Castiglione, Chem. Eur. J., 2023, 29, e202302025.

Invited Talk

In Silico Design and Characterisation of Thiophene-Based Materials for Organic Electronics

Mosè Casalegno, Politecnico di Milano, Italy

Abstract:

Thiophene plays a fundamental role in the development of semiconducting materials for organic electronics. Thienobelts are novel thiophene-based compounds obtained by wrapping up linear thienoacenes into belt-shaped structures. Here, ab initio calculations are used to provide preliminary insights into their structural and electronic properties. We find that belt-shaping significantly impacts these properties with respect to those calculated for linear thienoacenes. Our analysis suggests that thienobelts can be classified as organic semiconductors, but also reveals significant differences among them. Small thienobelts are aromatic and characterised by poor optical absorption properties, whereas large ones display the opposite behaviour. Based on this outcome, we identify two compounds that may deserve attention as synthetic targets.

INVITED TALK

Reconfigurable Electronic Structures in 2D vdW Heterostructures: Moiré, Stacking, and Strain via DFT/GW

*Hung-Chung Hsueh*1 and Chih-En Hsu1*

1Department of Physics, College of Sciences, Tamkang University, New Taipei City 251301, Taiwan

Abstract:

Reconfigurable band structures and excitons in 2D van der Waals materials provide a basis for non-volatile memories, ultra-low-power logic, and quantum/optoelectronic sensors. Within a unified GW/DFT/DFPT/BSE framework, we show how moiré patterning, stacking, strain, and composition act as design knobs for device functionalities. In CVT-grown multilayer $SnS_{1-x}Se_x$ ($0 \leq x \leq 1$), composition-controlled in-plane anisotropy in band gaps and thermoelectric coefficients enables polarised IR photodetectors, directional modulators, and integrated cryogenic thermoelectric coolers [1]. Epitaxial moiré h-BN/graphene heterostructures, with ABB/ABN stacking and electrically switchable out-of-plane ferroelectric polarisation, are promising for non-volatile ferroelectric tunnel junctions and neuromorphic synaptic elements [2]. Strain-stabilised chiral bilayer germanene on Ag(111) demonstrates that substrate and stacking engineering can define robust, spin–orbit–rich Xene channels for nanoelectronics[3]. Finally, large-scale GW–BSE simulations of Wigner

crystalline excitons in angle-aligned $MoSe_2/MoS_2$ moiré superlattices reveal long-lived, strongly correlated dark excitons whose real-space profiles follow generalised Wigner crystals [4], suggesting excitonic information processing and ultrasensitive, moiré-based quantum sensing via photocurrent tunnelling microscopy.

Reference:

[1] Thalita Maysha Herninda, et al., Mater. Today Advs. 18, 100379 (2023).

[2] Sheng-Shong Wong, et al., Advanced Materials, 2414442 (2025)

[3] Ting-Yu Chen, et al., Phys. Rev. B 112, L161406 (2025).

[4] Jing-Yang You, et al., PNAS (2026) (accepted)

INVITED TALK

Computational Optimisation of Functional Materials for Energy and Environmental Applications

Abdullah Alghafis

Associate Professor, Department of Mechanical Engineering, College of Engineering, Qassim University, Saudi Arabia

Abstract

The increasing global demand for efficient, reliable, and sustainable energy systems has intensified the need for advanced functional materials with carefully tailored physical, thermal, and structural properties.

Materials employed in energy and environmental applications, such as energy conversion devices, thermal management systems, and resource sustainability technologies, must satisfy complex and often competing performance requirements. Traditional experimental approaches to material development are time-consuming and costly, particularly when large multidimensional design spaces are involved. As a result, computational methodologies have become essential tools for accelerating material screening, evaluation, and optimisation. Nevertheless, many existing computational approaches rely either on high-fidelity numerical simulations with significant computational expense or on data-centric strategies that lack explicit physical interpretability, limiting their reliability when applied to novel material systems or under constrained data availability. This work presents a physics-guided computational optimisation framework for functional materials intended for energy and environmental applications.

The proposed framework integrates physically meaningful material descriptors representing structural features, thermal behaviour, and intrinsic material properties within a unified

computational workflow designed to guide performance prediction and material selection. Rather than treating material behaviour as a purely abstract input–output relationship, the framework emphasises established physical relationships in shaping model structure and parameter selection. This approach improves robustness, enhances generalisation across material classes, and reduces sensitivity to limited or sparse datasets, which are common in energy-related materials research. The framework is demonstrated through a representative case study involving functional materials relevant to energy systems. Key performance indicators associated with energy efficiency, stability, and operational effectiveness are evaluated across a multidimensional design space. Sensitivity analysis is employed to assess the relative influence of individual descriptors on overall performance, enabling transparent interpretation of material behaviour and supporting rational design decisions. The results indicate that the proposed framework achieves improved predictive consistency and reduced computational complexity compared to conventional optimisation strategies, while maintaining physical plausibility throughout the explored parameter space. Beyond performance evaluation, the framework facilitates rational material optimisation by identifying trade-offs between competing properties that are critical in energy and environmental applications. This capability is particularly valuable during early-stage material development, where experimental data are limited and exploratory insight is essential. The generality of the framework allows it to be adapted to a wide range of functional materials and energy-related applications, including thermal energy systems, energy harvesting technologies, and environmentally responsive materials. In summary, this study demonstrates that physics-guided computational optimisation provides a viable and scalable pathway for advancing functional materials for energy and environmental applications.

By combining physical understanding with computational efficiency, the proposed framework supports informed material selection and design, contributing to the development of sustainable energy technologies while maintaining scientific transparency and methodological rigour.

Keywords: Functional Materials; Energy Materials; Computational Optimization; Physics-guided Modelling; Environmental Applications

---

INVITED TALK

DFT Insights into Opto-electronic Properties of Near Infra-red (I) absorber 1:1 Perylene: TCNQ Cocrystal Towards Photovoltaic Application

Arkalekha Mandal,a Chris Erik Mohna, Yusuf Chanchangi,b Javier Carmona Garcia,c Carl Henrik Görbitza*

a Department of Chemistry, Blindern Campus, University of Oslo, Oslo 0371, Norway

b Environmental and Sustainability Institute, Faculty of Environment, Science and Economy, University of Exeter, Exeter, Penryn Campus, Cornwall TR10 9FE, United Kingdom

c School of Chemistry, University of Bristol, Clifton, Bristol, BS8 1TS, United Kingdom

Abstract

Organic cocrystals comprising π-electron-rich donors and π-electron-deficient acceptors hold immense potential for thin film photovoltaic devices for strong and broad optical absorption covering the visible and near-infrared region, intrinsic semiconductor property, and solution processing ability at ambient conditions, yet they are under-represented as photovoltaic materials. Herein, we investigated excited-state features and electron/hole transport properties of the cocrystal of π-donor perylene and π-acceptor 7,7′,8,8′-tetracyanoquinodimethane (TCNQ). The donor and acceptor molecules form infinite π-stacks via strong π··π stacking interactions to facilitate charge transfer. The absorption spectrum of this cocrystal shows broad absorption in the near-infrared region owing to charge transfer. A Time-dependent DFT study indicates efficient charge transfer, exciton generation and dissociation. The bandgap of the cocrystal (0.92 eV) is ideal for photovoltaic properties, while the theoretically calculated spectroscopic limited maximal efficiency (SLME) is 24 % at 1000 nm thickness, giving indication of practical applicability. The electron (45 meV) and hole (48 meV) transfer integral values along the π··π stacking direction indicate ambipolar charge transport, while low values of the internal reorganisation energy of perylene (147 meV) and TCNQ (255 meV) are favourable for fast transport of charge carriers, making the cocrystal suitable for photovoltaic applications. The perylene: TCNQ cocrystal poses an intriguing example of organic indirect bandgap material having high value of theoretical photovoltaic efficiency at low film thickness, owing to very similar values of indirect bandgap and direct allowed bandgap. This study unveils the photo-physical and charge transport properties of an organic cocrystal with strong potential for photovoltaic application.

INVITED TALK

Applications of Distributed Atomic Polarizabilities in Quantum Crystallography

Piero Macchi

Department of Chemistry, Materials and Chemical Engineering

Politecnico di Milano via Bassini 6, 20131 Milano

Abstract:

In this talk, we systematically investigate how to decompose the total polarizability of a molecule/solid into chemically meaningful atomic contributions. By comparing different partitioning schemes, we will reveal the strong dependence of atomic polarizabilities on the chosen method and emphasise the great potential of polarizability density—particularly its trace—as an analytical tool for studying molecular recognition and reactivity.

This method could be used to rapidly evaluate some material properties and to study secondary interactions, offering new insights for understanding and predicting the behaviour of molecular adducts, such as electron donor–acceptor complexes.

ORAL TALK

From Elemental Powders to Industrial Forging: FEM-Assisted Processing and Microstructural Evolution of PM U720Li Nickel-Based Superalloy

Wiktoria Skonieczna1, Marek Wojtaszek1, Kamil Cichocki1, Oleksandr Lypchanskyi1,2, Grzegorz Ficak1,3, Mike Gude4 und Ulrich Prahl5.*

1 AGH University of Krakow, Faculty of Metals Engineering and Industrial Computer Science, al. Adama Mickiewicza 30, 30-059 Kraków, Poland

2 Chemnitz University of Technology, Institute of Materials Science and Engineering, 09107, Chemnitz, Germany

3 GK FORGE SP Z O.O., ul. Przemysłowa 10, 43-440 Goleszów, Poland

4 Dresden University of Technology, Institute of Lightweight Engineering and Polymer Technology, Holbeinstr. 3, 01-307 Dresden, Germany

5 Institute of Metal Forming, Technische Universität Bergakademie Freiberg, Bernhard von Cotta Straße 4, 09599, Freiberg, Germany

Abstract:

Nickel-based superalloys are widely used in aerospace and energy industries due to their excellent mechanical properties and microstructural stability at elevated temperatures. Among modern manufacturing approaches, powder metallurgy combined with hot forming processes offers significant potential for tailoring the microstructure and improving the performance of these materials. However, optimisation of thermomechanical processing parameters remains a major challenge, particularly under industrial forging conditions.

The present work focuses on the analysis of hot forming and microstructural evolution of the U720Li nickel-based superalloy manufactured from elemental powders. The feedstock material was prepared by high-energy mixing in an Attritor mill followed by pressure-assisted consolidation. Plastometric tests were performed in the temperature range of 950–1200°C and strain rates from 0.1 to 20 s^{-1} in order to develop flow curves and processing maps describing the hot workability of the investigated alloy. The obtained rheological data were implemented into QForm UK software to perform FEM simulations of the industrial forging process. Numerical modelling enabled the prediction of strain and temperature distributions and supported the selection of process parameters for industrial trials conducted using a 400-ton screw press. Detailed microstructural characterisation, including SEM and EBSD analysis, revealed a clear relationship between local deformation conditions and

microstructural evolution. Regions subjected to higher strain exhibited grain refinement and features characteristic of dynamic recrystallisation, while low-strain regions retained partially deformed microstructures.

The results demonstrate that the integration of plastometric testing, processing maps and FEM simulations provides an effective approach for designing industrial hot forging processes of powder-metallurgy nickel-based superalloys and enables the production of high-quality forged components with controlled microstructure.

ORAL TALK

Colloidal Processing of Hydroxyapatite-Based Bioactive Ceramics Derived from Phosphate Rock for Bone Regeneration Applications

Sara M. Barroso Pinzón[1], Álvaro J. Castro Caicedo[1], Antonio Javier Sánchez-Herencia[2], Begoña Ferrari[2], Ana Ferrández-Montero[2]

[1] Universidad Nacional de Colombia, Facultad de Minas, Sede Medellín, Medellín, Colombia

[2] Instituto de Cerámica y Vidrio (ICV), Consejo Superior de Investigaciones Cientificas (CSIC), 28049 Madrid, Spain

Abstract

The development of bioactive ceramic scaffolds for bone tissue engineering requires not only appropriate chemical compositions but also robust and reproducible processing routes that enable precise control over architecture and porosity. In this context, hydroxyapatite-based systems remain widely investigated due to their chemical affinity with bone mineral; however, their processing into complex three-dimensional architectures remains challenging, particularly at high ceramic loadings. In this work, hydroxyapatite powders were synthesized by chemical precipitation using phosphate rock as a natural precursor of calcium and phosphorus, enabling the incorporation of trace elements such as magnesium and strontium, together with secondary calcium phosphate phases associated with magnesium-containing whitlockite. The synthesized powders exhibited nanometric particle size, high specific surface area, and enhanced surface reactivity, making them suitable for colloidal processing. The powders were subsequently processed through colloidal routes involving surface modification with polyethyleneimine (PEI) and dispersion within a polylactic acid (PLA) matrix. Under optimized processing conditions, the suspensions were shaped by tape casting to obtain uniform ceramic–polymer films and further processed by extrusion to produce composite filaments suitable for fused deposition modeling (FDM). These filaments enabled the fabrication of three-dimensional scaffolds with controlled porosity and interconnected architectures.

Overall, the results demonstrate that the integration of tailored powder synthesis with controlled colloidal processing provides a versatile and scalable route for the fabrication of

hydroxyapatite-based bioactive ceramic scaffolds via conventional forming and additive manufacturing techniques, highlighting strong correlations between powder characteristics and final scaffold architecture.

Keywords— additive manufacturing, bioactive ceramics, colloidal processing, hydroxyapatite.

ORAL TALK

Computational Reactivity Strategies Applied to Fullerene Derivatives in the Stabilisation of Hybrid Perovskite-based Solar Cells

Bruno Hori Barboza*1,2, Jules Harran2, Bryan Khemiri2, Orisson Ponce Gomes2, Augusto Batagin-Neto1, Didier Bégué2, Roger Clive Hiorns2

1 Universidade Estadual Paulista (UNESP-POSMAT/Brazil), 2 CNRS/Université de Pau et des Pays de l'Adour (UPPA-IPREM/France)

Abstract

Perovskite solar cells (PSCs) have achieved high efficiency over the past few years. However, despite the outstanding performance, inherent instability is an obstacle that hinders large-scale applications. In this context, polyfullerenes derivatives are a promising candidate to improve perovskite-based solar cells due to their good processability, optical and electrical properties and have already improved both efficiency and stability of organic solar cells. However, systematic studies are still necessary to clarify the associated processes and identify suitable derivatives. In this report, we explore predictive aspects of combined quantum mechanical descriptors (QMD) and molecular dynamics (MD) simulations to investigate the reactivity of a series of organic molecules and propose an analysis of the PF derivatives and the interactions with typical ionic species of hybrid perovskites and PSC interfaces.

In this sense, frontier molecular orbital levels and Fukui functions can predict orbital-driven interactions, whereas molecular electrostatic potential describes physisorption interactions where orbital overlap is negligible. However, no single descriptor fully predicts the reactivity, especially in the context of molecule flexibility or solution environments. In fact, a combined QMD and MD approach provides a more realistic description of chemical behaviour through thermodynamic, conformational changes and steric effects.

Understanding the details regarding the orbital, electrostatic, thermodynamic, and steric interactions provides insights about how poly(fullerene)s participate in the charge transfer process on solar cell devices. The results provide a perspective on how the combined molecular modelling techniques can contribute to the development of efficient and durable PSC photovoltaic devices.

Acknowledgements: CAPES - Finance Code 001 (Proc. 88881.218890/2025-01, 88887.933010/2024-00),

FAPESP (Proc. 2025/09784-1) and European Horizon program: HORIZON-CL5-2024-D3-01-02-EFFECTOR10117280

ORAL TALK

Oxygen vacancy-triggered electron traps and observation of a giant dielectric constant in hot-pressed perfectly dense calcium manganese oxide ceramics

Megha Pant1 and Ajit K. Mahapatro1,2*

1Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India; 2Department of Physics and Astronomy, University of the Western Cape, Bellville, South Africa

Abstract

The study of electronic charge transport processes prevalent in a material is essential for deciphering its potential for device applications in the technologically advanced industries. In this work, perfectly dense hot-pressed ceramics of highly pure calcium manganese powders ($CaMnO_3$) are prepared by optimising the ball-milling time and calcination temperature. The minimum time required for preparing highly pure and uniformly distributed sub-micrometre-sized $CaMnO_3$ features is attained by ball milling the precursor mixture of calcium carbonate and manganese dioxide for 12 h, followed by calcination at 1273 K for 2 h. Relative density of 99.03% is exhibited by the ceramics hot-pressed at 1073 K for 30 min. The electrical measurements pursued in the temperature range of 133-373 K through the optimised $CaMnO_3$ ceramics are fitted with a proposed model of hopping and trap charge-limited current conduction. The temperature-dependent trap density estimated as a fitting parameter is observed to reduce with increasing temperature. The energetic distribution of traps is estimated using frequency-dependent capacitance spectra. A giant dielectric constant ~ 106 is achieved in the temperature range of 133-593 K and frequency range of 1 Hz-20 MHz. Nyquist plots are fitted with an equivalent circuit model corresponding to contributions from grains and grain boundaries. AC conductivity is fitted with Jonscher's power law for estimating the dc conductivity and crossover hopping frequency. The presence of traps attributed to the origin of oxygen vacancies and the formation of polarons triggers electronic events interesting to thermoelectric and charge storage applications.

DAY – 2 ROOM -A

Session: Advanced Functional Materials

Keynote Talk

Sustainably Engineered N-Doped Carbon Dots: Structure–Property Modulation for Advanced Photoredox Applications and Light–Matter Interactions

Mariacecilia Pasini 1, Benedetta M. Squeo 1, Francesca Villafiorita-Monteleone 1, Federico*

Turco 1, Eleonora S. Cama 1, Chiara Botta 1, Umberto Giovanella 1

Istituto di Scienze e Tecnologie Chimiche 'Giulio Natta', Consiglio Nazionale delle Ricerche -

CNR-SCITEC, Via A. Corti, 12Milan, Italy

Presenter Mariacecilia Pasini

Abstract:

Organic and hybrid technologies increasingly require sustainable, multifunctional materials capable of operating across optical, electronic, and biological environments. Among emerging carbon-based nanomaterials, nitrogen-doped carbon dots (N-CDots) stand out for their tunable optoelectronic properties, low toxicity, water processability, and scalable synthesis, making them promising candidates for next-generation photonic, optoelectronic, agritech, and catalytic systems.

In this work, N-CDots synthesised through environmentally friendly routes were structurally and spectroscopically characterised (AFM, TEM, FT-IR, UV–Vis, PL), revealing controlled nanostructure, abundant surface functionalities, and excitation-dependent emission.

Incorporation of a nitrogen source, such as urea or polyethylenimine, enables modulation of nitrogen content, surface dipoles, and π-conjugation, yielding enhanced light absorption, red-shifted photoluminescence, and improved charge-transfer capability.

As UV-filtering additives, N-CDots provide adjustable transparency with high photostability. As interfacial modifiers in organic optoelectronics, they act as efficient charge-regulating layers. In non-fullerene Organic PhotoVoltaic devices (OPVs), N-CDots promote electron extraction by lowering the cathode work function and improving interfacial energetics. Their combination with PDINN (perylene-diimide-bearing aliphatic amines) results in synergistic effects, increasing short-circuit current density (Jsc), open-circuit voltage (Voc), fill factor, and operational stability.

Beyond optoelectronics, agritech studies demonstrate that N-CDots stimulate seed germination, radicle elongation, hydroponic growth, stomatal conductance, and water-stress recovery, monitored via in-plant bioristor sensing. In photoredox catalysis, N-CDots efficiently reduce methyl viologen under visible light, highlighting strong electron-donating behaviour relevant to hydrogen-evolving reactions.

Overall, the sustainable synthesis and tunability of N-CDots enable their deployment as multifunctional nanomaterials bridging optoelectronics, photonics, agritech, and photocatalytic technologies.

Keynote Talk

Cellulose: an ancient material for innovative applications

Paola Costanzo, Loredana Maiuolo, Vincenzo Algieri, Antonio Jiritano, Federica Meringolo, Antonio De Nino*

Abstract:

Cellulose, the most abundant biopolymer on Earth, has excellent potential to reduce our reliance on fossil feedstocks for the production of materials, in line with the UN Sustainable Development Goal 12. Thanks to its renewability, biodegradability, low toxicity, and high mechanical properties, cellulose is an ideal candidate for producing environmentally friendly and cost-effective polymeric products. Despite being one of the most ancient materials used by humans, cellulose still represents a significant challenge from both a chemical and environmental point of view, due to its poor solubility and reactivity. Chemical modifications allow for fine-tuning and enhancement of its properties, enabling its use in diverse fields. In recent years, many new cellulose-based materials have been developed not only as catalysts but also for water remediation and the development of biocomposites. In particular, chemically modified cellulose materials will be obtained by our research group as powerful tools for water purification from dyes, organic pollutants, and fuels. Furthermore, a novel series of bio-based cellulose composites has been designed with interesting mechanical properties for applications in building, packaging, and pharmaceuticals. Results from our investigations on cellulose derivatives will be presented, highlighting their versatility in these fields.

Keynote Talk

Refractory high-entropy alloys resistant to multicomponent aggressive gas mixtures

Zbigniew Grzesik1, Grzegorz Smola1, Richard Gawel1, Grzegorz Moskal2*

1AGH University of Krakow, Poland, 2Silesian University of Technology, Poland

Abstract

The variety of aggressive high-temperature gas atmospheres commonly present in several branches of technology results in a lack of a single universal metallic material capable of ensuring protection against corrosion under all conditions [1-3]. The main reason behind this

is the fact that currently used oxygen-resistant chromia or alumina-forming alloys undergo rapid corrosion in atmospheres containing other aggressive gases, e.g., sulfur [4]. Up to now, the prevalent opinion is that it is not possible to manufacture such materials. Consequently, it is necessary to precisely select alloy compositions for operation in specifically identified corrosive atmospheres.

The possibility of changing this situation is being discussed. Experimental results obtained in the last few years strongly suggest that thanks to the development of refractory high-entropy alloys, the opportunity has arisen to select a composition capable of resisting various aggressive gases to a degree comparable with that of several traditional materials currently used in individual gas environments. These alloys can be resistant not only to oxidation in a wide temperature range [5], but also to sulfur (S2, SO2) and water vapour attacks. Studied refractory high entropy alloys in oxygen and sulfur vapour-containing atmospheres degrade approximately in accordance with the parabolic oxidation rate law, and the determined parabolic oxidation rate constant values at 1000 oC remain at the level of 10-11 g2cm-4s-1. In addition, these alloys do not have to be obtained by arc furnace melting but can be synthesised much more cheaply at temperatures around 1000 oC.

1. Birks N., Meier G.H, Pettit F.S., Introduction to the high temperature oxidation of metals.

University Press, Cambridge, 2009.

2. Young D.J., High temperature oxidation and corrosion of metals. Elsevier. Amsterdam, the Netherlands, 2008.

3. Xu, H., Guo, H., Gong, S., Developments in High-temperature Corrosion and Protection of Materials. Woodhead Publishing in Materials, Cambridge, England, 2008.

4. Mrowec S., Oxidation of Metals, 44 (1995) 177-209.

5. Gorr B., Müller F., Schellert S., Christ H-J., Chen H., Kauffmann A., Heilmaier M., Corrosion Science, 166 (2020) 108475.

INVITED TALK

Hierarchically porous inorganic materials for efficient heterogeneous catalysis

Haifei Zhang and Binhang Zhao*

*Department of Chemistry, University of Liverpool, Liverpool, UK **

Abstract

Solid catalysts provide essential advantages, e.g., high reusability, easy separation, reducing equipment corrosion, in green chemistry and sustainable catalysis. Porous inorganic materials

with high surface areas and micro/mesoporous structures have been widely investigated. However, the lack of macropores in these materials hinders the efficiency of heterogeneous catalysis, particularly in viscose systems or involving large reaction molecules.

In this presentation, we report the preparation of hierarchically porous silica materials by ice templating and emulsion-templating techniques, using silica colloids and zeolite particles as building blocks. These materials contain mesopores and highly interconnected macropores. The acid groups are introduced by grafting of mercaptopropyl trimethoxysilane and subsequent oxidation using H2O2 under mild conditions. These porous solid acid catalysts show excellent conversion and recyclability as demonstrated with esterification and acetalization reactions.

INVITED TALK

Multi-material L-PBF of Ti-42Nb/Ti-5553 layered composites for enhanced strength and ductility

*João Felipe Q. Rodrigues1, Rubens Caram1**

1University of Campinas, School of Mechanical Engineering, Campinas, SP, Brazil

Abstract

Improving the mechanical response of load-bearing materials has traditionally focused on increasing strength, ductility, and toughness. Nevertheless, these properties are intrinsically interdependent: gains in strength are commonly accompanied by losses in ductility, and vice versa, a well-established limitation referred to as the strength–ductility trade-off. An effective approach to mitigate this constraint is the design of graded or layered architectures that integrate distinct materials, thereby promoting improved ductility and toughness without compromising strength. Laser Powder Bed Fusion (L-PBF), an additive manufacturing process in which components are produced layer by layer from metallic powders, provides a distinctive advantage: the possibility of tailoring chemical composition throughout the sample. This flexibility makes L-PBF especially suitable for the fabrication of architected and multi-material systems. In the present study, composite structures consisting of alternating layers of Ti-based alloys (Ti-42Nb and Ti-5553) were manufactured using a multi-material L-PBF platform. When subjected to aging treatments that induce α-phase precipitation within a β-phase matrix, Ti-5553 develops high mechanical strength. In contrast, Ti-42Nb, owing to its elevated solute content, displays moderate strength combined with remarkable ductility, primarily due to its limited responsiveness to aging treatments. The experimental results demonstrated the successful production of dense, defect-free layered structures. Vickers hardness and elastic modulus measurements indicated clear variations as a function of phase constitution and chemical composition. Tensile testing of the Ti-42Nb/Ti-5553 layered composites revealed that aging treatments strengthened the Ti-5553 layers while

simultaneously solution-treating the Ti-42Nb layers, ultimately yielding a material system that effectively combines high strength with good ductility.

INVITED TALK

Cobalt Ferrite Nanochessboard

Abdellah Lisfi

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

Abstract

In this study, we report the discovery of a cobalt ferrite nanochessboard with superior magnetic properties over the well-known CoFe2O4 inverted bulk phase. The patterned structure was stabilized in thin films through an epitaxial growth of CoFe2O4 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 emu/cm3), much higher than that yielded by the fully inverted phase of single crystal CoFe2O4 (400 emu/cm3). 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 Fe3+ and Co2+, their repartition among tetrahedral and octahedral sites and the magnitude and the sign of the anisotropy of Co2+ 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.

INVITED TALK

The Effect of Silicon Carbide Nanoparticles on the Plasticity and Microstructure of the PM Udimet 720LI Superalloy

Marek Wojtaszek1, Wiktoria Skonieczna1, Piotr Ledwig1, Kamil Cichocki1, Dariusz Zientara2, Mathias Zapf3 and Ulrich Prahl3.*

1 AGH University of Krakow, Faculty of Metals Engineering and Industrial Computer Science, al. Adama Mickiewicza 30, 30-059 Kraków, Poland

2 AGH University of Krakow, Faculty of Materials Science and Ceramics, al. Adama Mickiewicza 30, 30-059 Kraków, Poland

3 Institute of Metal Forming, Technische Universität Bergakademie Freiberg, Bernhard von Cotta Straße 4, 09599, Freiberg, Germany

Abstract:

The present work focuses on the analysis of the hot formability of the U720LI nickel-based superalloy and this material modified by the addition of 3% by mass of silicon carbide nanoparticles. The materials for investigation were produced using a proprietary method involving relatively inexpensive elemental powders, employing high-energy mixing of powders followed by sintering under pressure. Materials with high relative density, free from defects, and characterised by a uniform chemical composition and homogeneous microstructure have been obtained. For both materials, multi-scale SEM/STEM analyses were carried out to determine the effect of introducing nanoparticles on the microstructural and phase changes occurring during the manufacturing process, particularly at the stage of pressure-assisted sintering. Significant differences were observed as a result of modifications to the chemical composition of the Udimet 720Li alloy. In the next stage, plastometric tests were carried out on both the alloy in its original state and after modification with nanoparticles, using a thermomechanical simulator of hot forming processes. The experiments were conducted at a wide range of temperatures and at a range of strain rates commonly used on industrial production lines. True stress-true strain curves were developed and used to analyse the response of materials as a function of deformation parameters. It has been demonstrated that the recommended parameters for the plastic deformation of the initial alloy are a combination of temperature ranging from 1050°C to 1150°C and a strain rate in the range of 1 to 20 s-1, because under these conditions the material exhibits stable plastic flow, high sensitivity to dynamic recrystallisation and forms a homogeneous, fine-grained microstructure. The effect of the presence of nanoparticles on the flow behaviour of the Udimet 720LI alloy was then determined, and the results obtained were correlated with microstructural analysis. Key changes in the microstructure of the Udimet 720LI alloy resulting from the introduction of SiC nanoparticles into the matrix during the manufacturing process were identified, and their influence on the hot deformation process was evaluated. Particular attention was focused on changes in plasticity and their causes. Due to the range of parameters adopted for the study, the obtained results can be applied during the design of industrial hot-forming processes of structural components made from Udimet 720LI alloy, both in its initial chemical composition and that modified with nanoparticles.

INVITED TALK

Mid-IR emission of Si-based microspheres: From vibrational emission to resonant-mediated superplankian emission.

Fernando Ramiro-Manzano1 and Roberto Fenollosa1, Moisés Garín2, Francisco Meseguer1*

1 Instituto de Tecnología Química (ITQ), Consejo Superior de Investigaciones Científicas-Universitat Politècnica de València, 46022, Valencia, Spain

2 GR-MECAMAT, Universitat de Vic - Universitat Central de Catalunya (UVIC-UCC), 08500, Vic, Spain

Abstract

Silicon-based microspheres can reach high temperatures under relatively low laser irradiation. The key feature is their small contact area with the substrate, ideally reduced to a single point, which limits heat dissipation through conduction. At moderate excitation, hydrogenated amorphous silicon microspheres exhibit a pronounced emission peak around 2000 cm-1. This emission is attributed to vibrational modes of silicon–hydrogen bonds. Above a certain irradiation threshold, thermal emission from the resonant structure of the spherical cavity emerges, accompanied by a phase transition to polycrystalline silicon. This transition is irreversible and results in the disappearance of the Si hydrides emission. The resonant peaks can be described in terms of Mie resonances, and in polycrystalline silicon microspheres, the radiative response is attributed to free-carrier emission. Remarkably, certain resonant modes in polycrystalline microspheres exhibit emission intensities exceeding the theoretical blackbody limit, owing to optical absorption cross-sections exceeding their physical dimensions. This super-Planckian behaviour highlights the role of resonant photonic effects in enhancing thermal radiation at the microscale. This structured emission could enable the development of compact mid-infrared light sources based on bottom-up fabrication approaches employing microspheres.

INVITED TALK

Interplay Between Energy Transfer, Exciton Dissociation and Triplet-State Dynamics in Quasi-Two-Dimensional $FAPbBr_3$ Perovskites

Vidmantas Gulbinas 1, Marius Franckevičius 1, Paula Baltaševičiūtė 1*

1Center for Physical Sciences and Technology, Vilnius.

Abstract

Quasi-two-dimensional (quasi-2D) perovskites are composed of varying-thickness inorganic layers separated by organic spacers. Owing to their enhanced environmental stability, tunable bandgap, and narrow emission spectra, these materials are highly promising for applications in solar cells, photodetectors, and particularly light-emitting diodes (LEDs). Strong quantum confinement and large exciton binding energies distinguish quasi-2D perovskites from their

3D counterparts. The excitonic behaviour in quasi-2D perovskites is highly sensitive to the layer thickness.

In this study, quasi-2D FAPEAPbBr$_3$ perovskites with systematically varied dominant layer thicknesses were prepared and investigated using time-resolved photoluminescence spectroscopy over a range of temperatures. These perovskites exhibit narrow emission bands in the visible spectral region, making them particularly attractive for LED applications. When synthesised, mixed-phase, various-thickness quasi-2D structures are formed. This structural heterogeneity significantly affects both absorption and luminescence characteristics. Moreover, the presence of heavy lead ions induces strong spin–orbit coupling, enabling fast intersystem crossing between singlet and triplet states. The investigation results reveal three primary processes governing the excited-state dynamics: exciton transfer, exciton dissociation, and triplet-state formation. At low temperatures, triplet states dominate the relaxation dynamics. As temperature increases, thermally activated triplet-to-singlet back-conversion mitigates the role of triplet states. Near room temperature, exciton dissociation becomes the dominant process, leading to rapid luminescence decay in 3D domains. This effect is less pronounced in quasi-2D structures with smaller 3D domains due to enhanced carrier confinement.

A detailed understanding of these relaxation pathways provides valuable insights for the design of more efficient quasi-2D perovskite materials and optoelectronic devices.

INVITED TALK

Core-Controlled Assembly Mechanisms of Virus-Like Particles

Monica Enculescu1,2, Anca Aldea1,2, Maria-Lorena Jinga1,2, Irina Tsvetkova2,3, and Bogdan Dragnea2,3*

1National Institute of Materials Physics (NIMP), Magurele, 077125, Romania

2International Center for Advanced Training and Research in Physics (CIFRA), Magurele, Romania

3Department of Chemistry, Indiana University, Bloomington, IN 47405, USA

Abstract

Virus-like particles (VLPs) are widely used in drug delivery and vaccine development. Assembling VLPs in vitro is used for studying the thermodynamics and kinetics of the assembling processes. Brome mosaic virus (BMV) is one of the simplest and most thoroughly studied plant viruses. The capsid of BMV is composed of 180 identical protein molecules, which are clustered into hexamers and pentamers on the surface. The capsid's diameter is about 28 nm and has an 18 nm inner cavity. These capsids can be used for specific and localised treatment; therefore, it is important to study the thermodynamics of their assembling

processes. Thus, gold nanoparticles (GNP) with diameters that can be controlled from the synthesis were used as a cargo model.

For incorporation of gold nanoparticles into the viral capsid, the GNPs were functionalized with specific ligands which contain a hydrophobic alkaline chain with a thiol group on one side and a polyethene glycol chain with a carboxylic group on the other, ensuring the requirements for an assembly promoter: a negative surface charge for interaction with viral proteins, flexibility and hydrophilicity. The size of the gold particle has an influence on the structure of the resulting VLP and alters the yield of VLP emission. This study proposes the investigation of the influence of the GNP size on the icosahedral configurations of the VLPs and on the assembly mechanisms. For that, GNPs with different diameter values were used in fluorescence titration experiments to determine each phase in the assembly process.

Acknowledgements

The authors thank the National Authority for Scientific Research for the financial support through project PNRR Ctr. 760099/23.05.2023.

INVITED TALK

Polyester Hybrid Composites with Ceramic and Natural Fillers: Mechanical Performance and Thermal Behaviour

Merve Karaman*

İzmir Katip Çelebi University, Engineering Science Department, Çigli, İzmir, Türkiye

Abstract

In this study, polyester-based hybrid composites incorporating aluminium nitride (AlN) and a natural lignocellulosic filler were developed and systematically investigated. The total filler content was fixed at 40 wt.%, while the relative proportions of AlN and the natural filler were varied to evaluate their combined influence on composite performance.

Mechanical properties were determined through tensile and flexural tests. In addition, thermal characterisation analyses were carried out to evaluate the behaviour of the composites under elevated temperatures.

Fracture surfaces of tensile specimens were examined using scanning electron microscopy (SEM) to gain insight into filler dispersion, interfacial adhesion, and failure mechanisms within the composite structure. The results indicated that the incorporation of AlN and the natural filler significantly influenced mechanical properties and microstructural characteristics.

Overall, the hybrid filler system provided a tunable balance in composite performance, suggesting potential for applications where material efficiency and sustainability are of interest.

Oral Talk

Effects of Silver (Ag) Doping on Dielectric and Structural Properties of Polyethene Glycol (PEG) Nanocomposite Thin Films

Maria Naz1, Huseyin Furkan Eminoglu2, Deniz Bozoglu2, Deniz Deger2, Kemal Ulutas2, Sahin Yakut2

1 Istanbul University, Institute of Graduate Studies in Sciences, Turkey

2 Istanbul University, Faculty of Sciences, Department of Physics, Turkey

Abstract

Polyethene glycol (PEG) is a well-known biocompatible, thermoplastic, linear polymer. PEG has application potential in various areas, including drug delivery, coverage of biomedical devices, dermatological applications, and food packaging.

The structure to describe the nanocomposite of PEG including Ag is represented as Ag/PEG in this presentation. The variation of Ag doping ratio among thin film samples was defined as %10, %20, 30%, and %40 in terms of thickness. Ag/PEG nanocomposite thin films were deposited by a combination of thermal and electron beam deposition systems. 35000 g/mol PEG was selected as a thin film matrix, which was deposited by thermal evaporation. Ag granules with high purity were used as doping material, which was deposited by e-beam evaporation. Thicknesses of all samples were selected as 500 nm. Presence of Ag may cause a change in dielectric properties.

When dielectric results of pure PEG thin film are compared with Ag/PEG nanocomposites, it has been seen that at the low frequency side, where space charge polarisation can be observed, dielectric constants are almost the same for all samples. This can be attributed to the presence of a low amount of Ag atoms in nanocomposite thin films, which are polarised by accumulation at low frequencies. Toward higher frequencies, it has been seen that the dielectric constant differs for all samples. It can be evaluated as Ag atoms doped into the PEG thin film matrix were bonded to oligomers, which were produced as a result of the thermal evaporation process. Bonding of Ag atoms may cause restriction of segmental motion inside Ag/PEG nanocomposite thin films. Oligomers with changing sizes by the addition of Ag atoms can contribute to electric polarisation in dipolar characteristics.

DAY – 2, ROOM – B

Invited Talk

Session: Materials for Sustainable Energy, Environment and Nanotechnology

Controlling Ultrafast Photonic-Plasmonic Coupling in a Hybrid Platform for Biosensing Applications

Tersilla Virgili,1, Diego Florio,1,3 Laura Pasquardini,4,5 Mario Barozzi,6 Monica Bollani,1 Salvatore Stagira,3 Andrea Chiappini2*

1 Istituto di Fotonica e Nanotecnologia, CNR, P.zza Leonardo di Vinci 32, 20132 Milano, Italy

2 Istituto di Fotonica e Nanotecnologia, CSMFO Lab. and FBK Photonics Unit, via Sommarive 18, 38123 Povo (Trento), Italy

3 Politecnico di Milano, P.zza Leonardo di Vinci 32, 20132 Milano, Italy

4 Indivenire srl, via Sommarive 18, 38123 Trento, Italy

5 University of Campania Luigi Vanvitelli, Department of Engineering, via Roma 29, Aversa 81031, Italy

6 Fondazione Bruno Kessler, Sensors and Devices, via Sommarive 18, Trento, Italy Affiliation

Abstract

Photonic crystals are attractive for Surface-Enhanced Raman Scattering, biosensing, and waveguiding applications due to their ability to confine light in sub-wavelength regions and enhance near-field interactions at low fabrication cost. Their optical response is characterised by the presence of a photonic band gap (PBG), which governs light propagation through the periodic dielectric structure. When combined with plasmonic nanostructures supporting localised surface plasmon resonances (LSPRs), they form metal–dielectric hybrids (MDHs) with enhanced and tunable optical functionalities. Here, we fabricate an MDH featuring gold nanocaps (NCs) on the surface of a colloidal Photonic Crystal and characterise its optical response using static and femtosecond transient absorption spectroscopy. Static measurements reveal a broad plasmonic resonance in the near-infrared region, arising from the LSPRs sustained by the gold nanocaps. TA measurements uncover a strong interplay between the metal LSPRs and the opal PBG: the plasmon transient response is significantly enhanced by the PBG. For the first time, to the best of our knowledge, we demonstrate that this enhancement can be controlled by varying the excitation wavelength, owing to the slow-light regime, in agreement with predictions from the transfer matrix. Moreover, we show as proof-of-concept that the MDH ultrafast optical response is significantly modified by bacterial deposition, enabling ultrafast switching of the transient signal and underscoring the potential of these devices for biosensing applications1.

[1] Florio D. et al Advanced Optical Materials 2026, 10.1002/adom.202503745

Invited Talk

Advanced adsorbents for water remediation and critical raw materials recovery

Amerigo Beneduci

Department of Chemistry and Chemical Technologies, University of Calabria, Via P. Bucci 15D, Rende (CS) 87036, Italy

Abstract :

Water remediation and secure access to critical raw materials are often treated as separate challenges, yet both increasingly depend on the same enabling science: selective and sustainable separation in complex aqueous environments. In this context, adsorption is emerging not only as a simple and effective strategy for pollutant removal, but also as a key platform for recovering valuable elements from dilute secondary resources. This talk will highlight the potential of advanced adsorbent materials based on renewable cellulose and natural zeolites. Cellulose offers a versatile and sustainable scaffold whose surface chemistry can be tailored to control affinity, selectivity, and performance under realistic conditions. Natural zeolites complement this approach through their intrinsic porosity, ion-exchange capability, stability, and low cost, making them an attractive component for robust adsorbent systems.

Particular emphasis will be placed on how surface functionalization transforms these materials from passive sorbents into selective platforms for targeted separations, underscoring the broader opportunity to couple water treatment with the recovery of critical and strategic raw materials.

More broadly, the convergence of bio-based materials, natural minerals, and advanced interfacial design points toward a new generation of greener separation technologies aligned with circular-economy goals.

Invited Talk

APTES-Functionalized Kaolin–MgAl LDH Composite for Reactive Black 5 Adsorption

*Stavros G. Poulopoulos*1, Nargis, Xolmamatova1, Awal Adava Abdulsalam1, Ayobamiji Charles1*

1Nazarbayev University, Astana, Kazakhstan

Abstract

Reactive Black 5 (RB5) is one of the most commonly used reactive azo dyes in the textile industry. Dyes such as RB5 are toxic to humans and the environment if they are discharged

untreated into water bodies. Conventional treatment methods are insufficient in removing recalcitrant dyes. Clay-based composites have gained attention recently as low-cost and efficient adsorbents. Kaolin, a naturally abundant and chemically stable clay mineral, serves as an excellent support material. When combined with layered double hydroxides (LDHs), it enhances mechanical stability. Herein, kaolin-supported Mg–Al LDH (Kaolin–LDH) and 3-aminopropyltriethoxysilane (APTES)-functionalized kaolin-supported Mg–Al LDH (Kaolin–LDH–APTES) composites were synthesised and evaluated for RB5 adsorption from aqueous solution. The materials were characterised to confirm the successful formation of the composites and APTES grafting. Batch adsorption studies were performed to evaluate the effects of solution pH, competing ions, and natural organic matter (NOM) on RB5 removal. Results demonstrated that the Kaolin–LDH–APTES composite had almost double the capacity of the Kaolin–LDH composite. Kinetic studies revealed that the adsorption process for both materials followed the pseudo-second-order model, and equilibrium data were best fitted to the Langmuir isotherm. Effects of coexisting ions revealed that Na2SO4 had the strongest negative impact on RB5 removal for both composites, and humic acid, as the NOM model, showed a significant negative effect on the adsorption capacities of the composites. These findings demonstrate the potential of Kaolin–LDH–APTES as a low-cost and sustainable adsorbent for the treatment of reactive dye-contaminated wastewater under realistic environmental conditions.

Keynote Talk

Re-using wastes to improve asphalts in road pavements

Pietro Calandra1

** and Cesare Oliviero Rossi2*

1 CNR-ISMN Strada Provinciale 35D n. 9, Montelibretti (RM), Italy

2 University of Calabria, Arcavacata di Rende (CS)

Abstract

The construction and maintenance of road infrastructure traditionally impose significant environmental burdens, driven by high resource consumption and substantial landfill waste generation. To mitigate these impacts, recent studies investigate a circular economy framework integrating urban and industrial waste derivatives as high-value additives in asphalt manufacturing. The primary objective is to evaluate the feasibility of upcycling these sustainable residues to enhance the performance of neat bitumen, the key ingredient in road asphalts, and facilitate the recycling of reclaimed asphalt pavements (RAP). In this ambit, an excellent strategy turned out to be to thermally treat (pyrolysis) the wastes, so that a solid (char) and a liquid (pyro oil) can be obtained. A comprehensive rheological characterisation

determined the mechanical properties and evaluated the potential anti-ageing effects of the waste-enriched binders.

Experimental results indicate that the introduction of solid carbonaceous particles (as char) reinforces the intermolecular bitumen matrix, thereby increasing rutting resistance. Conversely, oils (also the pyrolytic oil fractions) act as effective fluxing and in some cases as real rejuvenating agents, restoring the viscoelastic properties of aged binders. Ultimately, dual-process integration demonstrates a viable pathway toward closed-loop pavement engineering, simultaneously reducing raw material dependency and diverting problematic waste streams from landfills.

Keynote Talk

Fifty Years of Goldene and a Gold Rush for Silicene and Further Xenes

Guy Le Lay

Aix-Marseille University, PIIM-CNRS

Abstract

The successful synthesis of the first artificial Graphene-like two-dimensional material, Silicene, by quantum design on a silver template, in 2012 [1], has launched a gold rush for the realisation of other mono-elemental atom-thin ones. Such new materials have appeared at a pace of about one per year, typically, from Germanene and Borophene in 2014 to Goldene in 2024, the first free-standing, flexible, noble metallene [2]. Standalone metallic Silverene has just been predicted by DFT calculations and ab initio molecular dynamics (AIMD) simulations [3,4]. Indeed, noble metallenes are extremely attractive for high-end applications, like in catalysis, plasmonics, sensing, electronics, and biomedicine [5]. I announced the birth of Silicene on an Ag(111) template 15 years ago in Dallas, Texas, at the 2011 March Meeting of the American Physical Society (APS). Antisymmetrically, just recently, in Denver, Colorado, at the March 2026 APS Global Summit, I could announce the birth of Silverene 'Through the looking glass', i.e., the other way around, after returning to my discovery of a Ge(111)6x6-Ag superstructure fifty years ago in 1976 [6]. This superstructure is due to an epitaxial silver ad-layer grown in situ under UHV on a germanium (111) substrate [7,8]. Scanning Tunnelling Microscopy/Spectroscopy observations/measurements at 4.4 K and associated Density Functional Theory calculations/simulations have now amazingly revealed a flat Kagome-derived Silverene sheet. In my talk, I will recall the iconoclastic struggle to achieve Silicene and the long march, 'Back to the Future', to obtain Silverene.

[1] P. Vogt, P. De Padova, C. Quaresima, J. Avila, E. Frantzeskakis, M.C. Asensio, A. Resta, B. Ealet, G. Le Lay, Silicene: Compelling Experimental Evidence for Graphenelike Two-Dimensional Silicon, Phys. Rev. Lett. 108 (2012) 155501.

[2] S. Kashiwaya, , Y. Shi, J. LU, D.G. Sangiovanni, G. Greczynnski, M. Magnusson, M. Andersson, J. Rosen, L. Hultman, Synthesis of goldene comprising single-atom layer gold, Nat. Synth. (2024) 1.

[3] E. J. A. dos Santos, R. A. F. Alves, A. C. Dias, M. L. Pereira, Jr., D. S.Galvaõ, and L. A.Ribeiro,Jr, Exploring Novel 2D Analogues of Goldene: Electronic, Mechanical, and Optical Properties of Silverene and Copperene, ACS Omega, 10 (2025) 26892.

[4] A. Zulfiqar, L. Xu, M. S. Arslan, Z. Huang, M. Zulfiqar, Z. Gu, Silverene: an atomically thin metallene with superior quantum capacitance, Surfaces and Interfaces, 72 (2025) 107452.

[5] S. Kashiwaya, Y. Shi, J. Rosen and L. Hultman, Perspectives on noble metallenes: from synthesis to application, 2D Mater., 12 (2025) 033001.

[6] G. Le Lay, G. Quentel, J.P. Faurie and A. Masson, Epitaxy of noble metals and (111) surface superstructures of silicon and germanium, Thin Solid Films, 35 (1976) 273.

[7] G. Le Lay, V.Yu. Aristov, L. Seehofer, T. Buslaps, R.L. Johnson, M. Göthelid, M. Hammar, U.O. Karlsson, S.A. Flodström, R. Feidenhasn'l, M. Nielsen, E. Finndeisen, and R.I.G. Uhrberg, STM and synchrotron radiation studies of "prototypical" metal/semiconductor systems, Surf. Sci., 307-309 (1995) 280.

[8] G. Le Lay, R.L. Johnson, R. Seemann, F. Grey, R. Feidenhans'l and M. Nielsen, Electronic and crystallographic structures of 2D silver adlayers on Ge(111), Surf. Sci., 287/288 (1993) 539.

Invited Talk

Effect of Benzoyl Peroxide on the Viscoelastic and Rheological Properties of LDPE Produced via Reactive Extrusion

*Nusret Kaya**

İzmir Katip Çelebi University, Faculty of Naval Architecture and Maritime, Naval Architecture and Marine Engineering, Çiğli, İzmir, Türkiye

Abstract

In this study, the viscoelastic behaviour of low-density polyethene (LDPE) modified with benzoyl peroxide (BPO) was systematically investigated. LDPE-based samples containing varying BPO concentrations (0.1%, 0.2%, 0.5%, and 1%, corresponding to 100, 200, 500, and 1000 ppm) were produced via melt extrusion. The primary objective was to evaluate the influence of peroxide-induced structural modifications on the mechanical, thermal, and rheological properties of LDPE, with particular emphasis on flow behaviour at 160 °C.

The rheological properties and linear viscoelastic behaviour of the samples were analysed using a rotational rheometer. Oscillatory tests were conducted to assess changes in storage modulus, loss modulus, and complex viscosity as a function of BPO content. Thermal properties were characterised by differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA), while structural and morphological features were examined using X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR).

The results indicated that the incorporation of benzoyl peroxide significantly altered the viscoelastic response of LDPE due to chain scission and/or branching reactions occurring during reactive extrusion. Increasing BPO concentration led to noticeable changes in melt flow behaviour, with implications for processability and material performance. Thermal analysis revealed modifications in crystallinity and thermal stability, while spectroscopic and diffraction analyses confirmed structural variations in the polymer matrix.

Overall, this study demonstrates that controlled peroxide modification is an effective approach to tailoring the rheological and thermomechanical properties of LDPE, offering valuable insights for optimising processing conditions and expanding application potential.

Invited Talk

pH-Thermo Dual-Responsive Polymeric Nanoparticles for Women's Health: Dual Action Against Cervical and Ovarian Cancer Cells

Filippo Rossi 1,, Giuseppe Nunziata 1 and Alberto Rainer 2*

1 Department of Chemistry, Materials and Chemical Engineering "Giulio Natta", Politecnico di Milano, 20133 Milan, Italy

2 Department of Engineering, Università Campus Bio-Medico di Roma, 00128 Rome, Italy

Abstract

The development of smart nanocarriers capable of responding to tumour-specific stimuli represents a promising strategy for improving therapeutic selectivity in oncology. In this work, we present a class of dual-responsive polymeric nanoparticles (NPs) engineered for precision drug delivery in gynaecological cancers. Amphiphilic block copolymers of the type P(MAA)-b-P(EG2MA-co-NIPAM) integrating pH-responsive methacrylic acid (MAA) and thermoresponsive diethylene glycol methylether methacrylate (EG2MA) and N-isopropylacrylamide (NIPAM) units were synthesised via reversible addition−fragmentation chain transfer (RAFT) polymerisation. Fine-tuning of the lower critical solution temperature (LCST) was achieved by modulating the ratio between NIPAM and EG2MA, yielding copolymers with cloud points within the physiologically relevant range of 30−40 °C. The resulting NPs exhibited sharp and reversible swelling/shrinking behaviour in response to pH and temperature stimuli, with sizes below 182 nm and narrow polydispersity indices. The

core−shell architecture was stabilised by a dodecyl-functionalized chain transfer agent, ensuring efficient self-assembly and robust encapsulation of both hydrophilic and hydrophobic drugs. Drug release studies with 5-fluorouracil (5-FU) and the drug-mimetic fluorescein isothiocyanate (FITC) confirmed a marked temperature-triggered release above the LCST and enhanced diffusion in mildly acidic conditions (pH < 6), characteristic of solid tumours. Cellular studies on HeLa and ovarian adenocarcinoma OVCA433 lines revealed rapid internalisation, high biocompatibility, and a significant increase in therapeutic efficacy of 5-FU when delivered via NPs, compared to the free drug. These findings highlight the potential of the dual-responsive nanoplatform for targeted and controlled delivery in the treatment of cervical and ovarian cancers.

ORAL TALK

Hierarchical Interfacial Engineering of BCZT/CFO Core-Shell Particles in PVDF Matrix: Surface Modification Strategy Toward High-Performance Magnetoelectric Composites for Piezoelectric Energy Harvesting

Chaymae Bahloul a, Sarah Baayyad a, Adil Eddiai b, Francisco Javier Romero c, Mohamed Rguiti d, Abou El Kacem Qaiss a, Fatima-Zahra Semlali a, , Rocío Moriche c,* and Mounir El Achaby a,**

a College of Chemical Sciences and Engineering (CCSE), Department of Materials Science, Energy and Nano-engineering (MSN), Mohammed VI Polytechnic University (UM6P), 43150, Benguerir, Morocco

b Laboratory of Physics of Condensed Matter (LPMC), Faculty of Sciences Ben M'Sik, Hassan

II University of Casablanca, Casablanca, Morocco

c Departamento de Física de la Materia Condensada, Facultad de Física, Universidad de Sevilla-ICMS, Avda. Reina Mercedes, s/n, 41012, Sevilla, Spain

d Univ. Polytechnique Hauts-de-France, INSA Hauts-de-France, CERAMATHS, F-59313, Valenciennes, France

Abstract

Achieving a balanced combination of magnetic, ferroelectric, and dielectric properties in flexible magnetoelectric polymer composites remains a significant challenge, particularly for energy harvesting applications. This work evaluates a surface modification strategy introduced at an intermediate stage of synthesis, where organic modifiers-oleic acid (OA) and polyvinylpyrrolidone (PVP)-are applied after BCZT core formation but before $CuFe_2O_4$ (CFO) shell growth. By placing the modifier directly at the BCZT/CFO interface, partial

redistribution toward the particle surface was allowed. This created a distinct interfacial configuration that differs fundamentally from conventional post-synthesis treatments.

The resulting BCZT/CFO core-shell particles were incorporated into a PVDF matrix via solution casting to produce flexible composite films. Their structural, morphological, thermal, and multifunctional properties were characterised via a suite of systematic tests. Compared to unmodified systems, both PVP- and OA-treated samples showed improved performance, though the extent of enhancement depends heavily on the specific modifier used.

Among the studied composites, the OA-modified system exhibits the most balanced response: remanent polarisation reached 0.49 μC.cm-2, saturation magnetisation hit 6.49 emu. g-1, and dielectric permittivity stayed around 30. These gains stem from superior particle dispersion and better compatibility with the polymer matrix. Crucially, the approach also appears to suppress unwanted magnetic interactions between particles. These findings demonstrate that introducing surface functionalization during synthesis, rather than after, directly influences the interfacial characteristics and multifunctional behaviour of magnetoelectric polymer composites.

ORAL TALK

NiO_x and CuO_x Thin Films Hole Transport Layers for Perovskite Solar Cells

Benjamín Atala-Niedmann1, Tamara Beltrán1, José Díaz1, Paola Sánchez1, Fernando Álvarez-Asencio1,2, Leonardo Vergara1,2, Ricardo Henriquez1, Valeria del Campo1*

1 Universidad Técnica Federico Santa María, Chile; 2 Pontificia Universidad Católica de Valparaíso, Chile

Abstract

Perovskite solar cells (PSCs) have emerged as a promising photovoltaic technology due to their rapid increase in power conversion efficiency and low-cost fabrication potential [1]. A key factor governing device performance is the hole transport layer (HTL), which strongly influences charge extraction, recombination, and long-term stability [2].

Conventional organic HTLs are costly and prone to degradation, motivating the development of scalable inorganic alternatives [3]. Nickel oxide (NiO_x) is widely studied due to its high transparency, favourable energy level alignment, and intrinsic stability. In addition, copper oxide (CuO_x) represents a promising HTL, offering comparable stability and compatibility with scalable deposition techniques such as sputtering, while being particularly attractive in copper-rich regions such as Chile [4].

In this work, we aim to develop and compare NiO_x and CuO_x thin films as inorganic HTLs for PSCs. Thin films are deposited by physical vapour deposition and sputtering, followed by

controlled oxidation, and characterised using optical, electrical, and morphological techniques. Additionally, a graphene-based interfacial layer is explored as a complementary strategy to suppress perovskite diffusion into the oxide and enhance interfacial stability and charge transport.

[1] J. Y. Kim et al., High-Efficiency Perovskite Solar Cells, Chemical Reviews, 2020.

[2] S. S. Mali et al., Role of Hole Transport Layer in Perovskite Solar Cells, Nanoscale, 2016.

[3] J. Tirado et al., Nickel Oxide as Inorganic Hole Transport Material, ACS Applied Energy Materials, 2019.

[4] A. Kumar et al., Thermally Oxidised Ultrathin Copper Film as Low-Cost HTL, Solar Energy, 2022.

Session: Online Session

Keynote Talk

Supramolecular Self-Assembly of Fullerenes: Zero to Higher Dimensions

*Lok Kumar Shrestha1,2**

1Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba 305-0044, Japan; 2Department of Materials Science, Institute of Pure and Applied Sciences, University of Tsukuba; 1-1, Tennodai, 305-8573 Tsukuba, Ibaraki, Japan

Abstract

Buckminsterfullerene (C60), an ideally zero-dimensional (0D) molecular nanocarbon building block, undergoes supramolecular assembly and forms various assembled nanostructures, including one-dimensional (1D) fullerene nanorods or nanotubes, two-dimensional (2D) nanosheets, and three-dimensional (3D) cubes at the liquid-liquid interface. These nanostructures result from the supramolecular assembly of fullerene molecules due to the π-π stacking interactions. These fullerene nanomaterials have emerged as novel π-electron-rich carbon sources for producing shape-controlled porous carbon materials in demand for sensing, energy storage, and energy conversion applications. In this contribution, we will discuss recent advances in the production of self-assembled fullerene crystals spanning zero to higher dimensions, including porous fullerene crystals with bimodal pore architectures and hierarchical superstructures composed of fullerene nanorods growing from a cubic solid core. We also discuss the direct conversion of these fullerene nanomaterials into hierarchically porous carbon materials with micro- and mesopore architectures via high-temperature carbonisation and their applications in energy storage and energy conversion. Finally, we will discuss the novel MOFOF and COFOF composite materials obtained by integrating coordination and supramolecular chemistry, as well as the derived metallic-nanoparticle-anchored carbon superstructures for energy-related applications.

Invited Talk

Tunable 3D Hybrid Nanocomposites for Adaptive Electromagnetic Shielding and Advanced Optoelectronic Applications

M. Suchea1,2, P. Pascariu1,2,3, C. Romanitan1, O. Brincoveanu1, C. Pachiu1, A.G.M. Popescu1, D. Manica1, M. Manica1, R. Marinescu1, I.V. Tudose1, A. Dinescu1, R. Muller1, O. N. Ionescu1 and E. Koudoumas1,2*

1National Institute for Research and Development in Microtechnologies (IMT-Bucharest), 023573, Bucharest, Romania

2Center of Materials Technology and Photonics, School of Engineering, Hellenic Mediterranean University, 71410 Heraklion, Crete, Greece;

*3Insititute of Macromolecular Chemistry, Petru Poni, Iasi, Romania **

Abstract

The rapid expansion of advanced communication systems and interconnected electronic platforms has intensified the need for materials capable of effective and adaptable electromagnetic interference (EMI) shielding. This invited presentation focuses on the development of tunable three-dimensional (3D) hybrid nanocomposites based on rare-earth-doped ZnO (RE: ZnO) integrated with graphene nanoplatelets, designed for both adaptive electromagnetic shielding and advanced optoelectronic functionalities.

The proposed approach exploits synergistic interactions between dielectric ZnO matrices and highly conductive graphene networks, while rare-earth dopants (e.g., La, Er, Sm) enable precise tuning of the electronic structure, carrier dynamics, and optical response. The resulting hierarchical 3D microstructures, fabricated via electrospinning–calcination techniques, exhibit high surface area, interconnected architectures, and controlled crystallinity. Comprehensive structural and spectroscopic investigations demonstrate strong correlations between dopant type, microstructural parameters, and electromagnetic performance.

The developed nanocomposites achieve shielding effectiveness values up to ~30 dB in the X-band, with dominant absorption-driven mechanisms, making them suitable for lightweight and efficient EMI mitigation. Beyond shielding, their tunable optical and electrical properties enable integration into optoelectronic devices, offering multifunctional performance within a single material platform.

These results highlight the potential of 3D hybrid nanocomposites as versatile and scalable solutions for next-generation adaptive electromagnetic management and high-performance optoelectronic applications.

Acknowledgement: This research was partially supported by PNRR/2022/C9/MCID/I8CF23/14 11 2022 contract 760101/23.05.2023 financed by the

Ministry of Research, Innovation and Digitalisation within the – PNRR-III-C9-2022 - I8 PNRR/2022/Component 9/investment 8 and partially supported by the Ministry of Education and Scientific Research through National Nucleus Programme μNanoEl, project code PN 2307, 8N/03.01.2023.

Invited Talk

Advances of Hydrodynamic Cavitation from an Informatics Point of View

*Máté Polgár1, Gábor Németh1, Levente Csóka2**

1Faculty of Wood Engineering and Creative Industries, Institute of Applied Sciences, University of Sopron, 9400 Sopron, Hungary

2ELTE Eötvös Loránd University, Faculty of Informatics, 1053 Budapest, Hungary

Abstract

In contemporary research, the boundary between computer science and the physical world has increasingly blurred, suggesting that information theory can describe fundamental natural processes, including quantum phenomena. Within this framework, a “bit change” represents the smallest unit of transformation, analogous to discrete transitions in nature. This talk examines hydrodynamic cavitation (HDC) as a physical tool to control bacterial quorum sensing by interpreting it as a molecular communication network.

Quorum sensing is a density-dependent signalling process in which bacteria exchange molecules such as N-acyl homoserine lactones to coordinate behaviour. From an information-theoretic perspective, these signals act as encoded bits transmitted through a noisy diffusion channel. Studies indicate that bacteria often employ a binary encoding scheme (1 bit), enabling efficient communication governed by Shannon entropy, which quantifies system randomness.

A key concept in this framework is the link between entropy and energy transformability: as entropy increases, the capacity for useful energy transformation decreases. Bacterial signalling systems exhibit non-negative entropy production, reflecting their dissipative and irreversible nature.

Hydrodynamic cavitation introduces localised high-energy events via collapsing microbubbles, disrupting signalling molecules and biofilm integrity. By increasing channel entropy, HDC effectively reduces cooperative information exchange. Viewing HDC as a controller of information flow enables optimisation strategies to suppress bacterial virulence and biofilm formation.

Invited Talk

Interfacially Engineered ZnO/Ti3C2Tx MXene Heterostructures for Enhanced Photocatalytic and Antibacterial Performance

Taghreed Al-Mutairi1,2, Ridha Hamdi2,3, Tahani Al-ghamidi2, M. Younas4, Hafedh Kochkar3,5*, Amor Ben Ali3,5 and Essam Kotb3,6*

1Department of Physics, College of Sciences, Qassim University, Saudi Arabia.

2Department of Physics, College of Science, Imam Abdulrahman Bin Faisal University, P.O. Box 1982, 31441, Dammam, Saudi Arabia.

3Basic & Applied Scientific Research Centre, Imam Abdulrahman Bin Faisal University, P.O. Box 1982, 31441, Dammam, Saudi Arabia.

4Department of Physics, College of Sciences, King Fahd University of Petroleum & Minerals, Dhahran, 31261, Saudi Arabia

5Department of Chemistry, College of Science, Imam Abdulrahman Bin Faisal University, P.O. Box 1982, 31441, Dammam, Saudi Arabia.

6Department of Biology, College of Science, Imam Abdulrahman Bin Faisal University, P.O. Box 1982, 31441, Dammam, Saudi Arabia.

Abstract:

In our work, optimised composition Ti3C2Tx MXene/ZnO heterostructures were prepared from Ti3C2Tx MAX phase precursor and studied for multifunctional environmental applications. Designing efficient semiconductor-based heterojunctions is recognised as a promising tool to exceed the charge recombination restrictions and promote the photocatalytic and antibacterial properties. A hybrid architecture containing conductive Ti3C2Tx MXene sheets together with ZnO nanoparticles was developed to accelerate the transfer of interfacial charges and improve the functional properties. The synthesised composites were characterised structurally, morphologically, and interfacially by X-ray diffraction (XRD), high-resolution transmission electron microscopy (HRTEM), selected area electron diffraction (SAED), X-ray photoelectron spectroscopy (XPS), and electrochemical impedance spectroscopy (EIS).

According to HRTEM and SAED analyses, ZnO nanoparticles were effectively glued by MXene basal planes without compromising the hexagonal Ti–C structure with the [0001] zone configuration. The heterostructures formed by those techniques exhibited close interfacial contact, which provides a favourable field for charge transmission and separation. The formation of covalent Ti–O–Zn bridging bonds at the heterointerface was verified by XPS analysis. These bonds serve as a chemical link between the two components to establish electronic communications over any interface and for electronic transmission. The increased interfacial interaction greatly enhanced charge-transfer kinetics as measured by the EIS

measurements. In particular, the optimised composite presented an outstanding reduction of the charge-transfer resistance from 131 MΩ to 5 KΩ and a rapid relaxation time of about 7 μs, which showed improved electron transport efficiency and suppressed charge recombination. Compared to the individual constituents, the optimised ZM5 heterostructure exhibited a higher multifunctional performance. Photocatalytic characterisation using formic acid, a known class of pollutants, showed a degradation rate of 58.7%, justifying the favourable influence of MXene-assisted charge separation.

Antibacterial studies demonstrated strong activity against Salmonella Enteritidis with inhibition zones of up to 16 mm. The improvement of photocatalytic and antibacterial activities by two times in this same model reveals the potential of combining techniques, such as interfacial engineering in MXene-based heterostructures. Based on these findings, chemically anchored ZnO/Ti3C2Tx heterostructures could serve as attractive multivalent materials for environmental protection and antimicrobial applications. ZnO and MXene exhibit a synergistic interaction, with that synergistic interaction offering a potential platform for exploring advanced materials, including improved charge transfer performance, pollutant degradation efficiency, and pathogen inactivation.

Keywords: MXenes; ZnO NPs; 2D heterostructures; Interfacial charge transfer; Ti-O-Zn covalent bonding; Photocatalysis; Antibacterial activity.

POSTER PRESENTATIONS

ME01 - Investigation of Quinoline Derivatives as Corrosion Inhibitors for AISI 430 Stainless Steel in Acidic Solution: Experimental and Theoretical Analysis

*Vitor Fernandes Moreno1,2,3 , Bruno Hori Barboza*1,3, Didier Bégué3, Augusto Batagin-Neto1, Roger Clive Hiorns3, Luiz Carlos da Silva Filho1*

1Universidade Estadual Paulista (UNESP-POSMAT/Brazil);

2Universidade de São Paulo (USP/Brazil),

3CNRS/Université de Pau et des Pays de l'Adour (UPPA-IPREM/France)

Abstract

The corrosion process leads to the degradation of metallic materials and imposes a significant economic impact on industrial production and maintenance. The use of inhibitors on stainless steel surfaces is a critical strategy for mitigating corrosion, particularly in aggressive acidic environments. In this context, quinoline derivatives have attracted interest due to their potential as corrosion inhibitors and are noteworthy as a versatile class of molecules, which allows a wide range of applications. In this report, we investigate the corrosion inhibitory properties of a group of quinoline derivatives on the surface of AISI 430 stainless steel through experimental and computational approaches.

Through the experimental, synthesis and electrochemical analysis were conducted to evaluate the inhibitory properties of quinoline derivatives towards the corrosion processes induced in coated AISI 430 steel samples, immersed in acidic solutions (HCl). To investigate the interaction process, a computational approach was performed through density functional theory (DFT) calculations and molecular dynamics (MD) simulations. The results indicate a significant corrosion inhibition rate (up to 99.45%), a factor that depends on the side groups attached to the quinoline rings, indicating that aminoquinolines are more effective inhibitors than nitroquinolines. From the computational aspects, DFT and MD simulations contributed to elucidating the mechanisms of interaction of the quinolines over the steel surface in solution and predicting the inhibitory properties of the selected derivatives.

Acknowledgements: CAPES - Finance Code 001 (Proc. 88881.218890/2025-01, 88887.933010/2024-00) and FAPESP (Proc. 2025/09784-1, 2024/14443-6).

ME02 - Texture Evolution and Elastic Modulus Tailoring in Additively Manufactured Ti-42Nb Alloy

João Felipe Queiroz Rodrigues1, Carlos Samuel Alves da Silva1, Hugo André Magalhães de Azevedo1, Matheus Valentim1, Márcio Sangali1, Rubens Caram1*

1University of Campinas, Brazil

Abstract

Additive manufacturing (AM) has emerged as a promising route for producing metastable β-Ti alloys for biomedical applications due to its capability to tailor microstructure and crystallographic texture. In this work, the texture evolution and elastic anisotropy of a Ti-42Nb alloy fabricated by laser powder bed fusion (LPBF) were systematically investigated through a combined experimental and computational approach. First-principles calculations based on Density Functional Theory (DFT) were performed using a Special Quasirandom Structure (SQS) BCC supercell in order to determine the single-crystal elastic constants and orientation-dependent elastic properties of the β phase. Young's modulus, bulk modulus, and shear modulus were obtained and used to construct elastic modulus orientation maps. Experimentally, the influence of LPBF scanning strategy on texture development was evaluated. Initially, a standard interlayer rotation angle of 67° was adopted while maintaining constant laser power, hatch spacing, and layer thickness. The scanning speed was varied between 400, 800, and 1200 mm/s to investigate its effect on crystallographic texture evolution. Subsequently, a lower scanning speed of 300 mm/s was selected to further evaluate the influence of different layer rotation angles, including 0°, 67°, and 90°. Electron Backscatter Diffraction (EBSD) analyses revealed significant changes in texture intensity and preferred crystallographic orientation as a function of the scanning strategy. By combining EBSD-derived texture data with the elastic properties obtained from DFT calculations, the effective Young's modulus along the building direction was quantified. The sample processed with a 90° rotation strategy exhibited a highly pronounced <001> fiber texture parallel to the building direction, resulting in the lowest elastic modulus of approximately 46 GPa. This value is remarkably close to the theoretical minimum modulus predicted for the β-Ti single crystal (~44 GPa), demonstrating the strong potential of texture engineering in LPBF Ti-Nb alloys for low-modulus biomedical applications.

[1] Pilz, S., Gustmann, T., Günther, F., Zimmermann, M., Kühn, U., & Gebert, A. (2022). Controlling the Young's modulus of a β-type Ti-Nb alloy via strong texturing by LPBF. Materials & Design, 216, 110516.

ME03 - Additive Manufacturing of Hybrid Titanium Alloys by PBF-LB: Controlled Microstructural Gradients and Mechanical Response

*Gilberto Vicente Prandi1 *, Mariana Sizenando Lyrio1, João Felipe Q. Rodrigues1, Matheus Valentim1, Virginie Roche5, Alberto M. Jorge Junior2,3,4, Rubens Caram1.*

[1]School of Mechanical Engineering – University of Campinas (UNICAMP) - Brazil, 2Graduate Program of Materials Science and Engineering, Federal University of São Carlos - Brazil. 3 Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, Institute of Engineering and Management, SIMAP – France,

4Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS,

Grenoble INP, Institute of Engineering and Management Univ. Grenoble Alpes, LEPMI – France

Abstract

Titanium alloys offer outstanding microstructural versatility, enabling components with tailored mechanical performance through compositional and processing control. Ti-42Nb retains a fully β-phase microstructure upon cooling, suppressing ω-phase formation and resulting in a low elastic modulus (~62 GPa) and excellent biocompatibility. In contrast, Ti-5Al-5Mo-5V-3Cr (Ti-5553) achieves high strengthening via α-phase precipitation and is widely applied in aerospace and marine sectors due to its toughness and corrosion resistance. Their combination provides a promising strategy for functionally graded materials with spatially controlled properties. This work explores the fabrication of Hybrid Titanium Alloys (HYTA) by laser powder bed fusion (PBF-LB). Prealloyed Ti-42Nb and Ti-5553 powders were blended at 80:20 wt.% under an inert atmosphere. Cylindrical specimens were produced using an OmniSint-160 system with a Yb: YAG fibre laser. Both homogeneous and graded samples were fabricated. Functional gradation was achieved by progressively increasing laser power (200–400 W) and adjusting scanning speed every 33 layers (~1 mm) to promote microstructural variation along the build direction. Microstructural characterisation was performed using FE-SEM, FIB cross-sections, EDS, EBSD, and X-ray microtomography. Mechanical behaviour was evaluated by Vickers microhardness (500 gf, 15 s) and compression testing (20 kN capacity, 1 mm/min). Results confirmed spatially distinct regions in graded specimens. Ti-5553-rich domains exhibited higher strength, while Ti-42Nb-rich regions preserved β-phase stability and reduced stiffness. Controlled laser parameter adjustment enabled either homogenised microstructures or sharply defined hybrid zones, demonstrating the feasibility of hybrid additive manufacturing for titanium components with spatially engineered mechanical performance for biomedical and structural applications.

ME04 - Tailoring Mechanical and Microstructural Properties of PBF-LB Ti-Nb-Ta Multilayer Composites for Biomedical Applications

Mariana Lyrio1, Gilberto Prandi1, Rubens Caram1*

1University of Campinas, School of Mechanical Engineering, Brazil

Abstract

The mechanical properties of titanium alloys can be tailored through precise adjustments in chemical composition and additive manufacturing, particularly Powder Bed Fusion - Laser Beam (PBF-LB). This technique enables the fabrication of dense, complex components with localised compositional variations. A critical challenge in orthopaedic implants is stress shielding, which occurs when a stiff metallic implant bears the majority of the physiological load, preventing it from being transferred to the surrounding bone. This lack of mechanical

stimulus leads to bone resorption and potential implant failure. Strategies such as multilayer or functionally graded processing (FGM) address this by combining regions of high strength with a low elastic modulus to match human bone stiffness. In Ti-Nb-Ta systems, Nb and Ta act as β-stabilizers; high concentrations stabilise the β-phase, significantly reducing the elastic modulus, whereas reduced contents favour martensitic transformation (α/α") to enhance strength. This study investigates multi-layered composites fabricated from Ti-xwt%Nb-6Ta (x = 20, 35) powders via PBF-LB. The structure consists of a Ti-35Nb-6Ta (600 μm) matrix and Ti-20Nb-6Ta (300 μm) reinforcement.

XRD confirmed the presence of martensitic phases alongside the β-matrix. SEM and EBSD analysed the α, α", and β phase distribution and crystallographic texture resulting from rapid solidification. Dilatometry identified the 450–600 °C range for thermal treatments to control precipitation. Hardness measurements revealed an intermediate gradient at the interface, confirming successful metallurgical bonding. This PBF-LB route offers a promising approach for patient-specific implants with an optimal balance of strength, stiffness, and biocompatibility.

ME05 - Alpha phase nucleation in a metastable beta Ti-Nb-Fe-Sn alloy: intergranular and intragranular precipitation mechanisms.

Leticia F. Starck1, Matheus Valentim1, Gilberto V. Prandi1, João Felipe Q. Rodrigues1, David Diercks2, Michael J. Kaufman3, Rubens Caram1*

1 University of Campinas, School of Mechanical Engineering, Campinas, SP, Brazil

2 Shared Instrumentation Facility, Colorado School of Mines, 80401, Golden, CO, USA

3 Department of Metallurgical and Materials Engineering, Colorado School of Mines, 80401, Golden, CO, USA

Abstract

Metastable b-Ti alloys are promising structural biomaterials due to their potential to combine low elastic modulus and high mechanical strength. These alloys are typically solution treated above the β-transus followed by rapid cooling to produce a predominantly β-phase microstructure with low elastic modulus that minimises the stress-shielding effect. Subsequent ageing is used to promote α-phase precipitation within the β matrix, thereby increasing strength. By controlling ageing parameters, it is possible to balance low modulus and high strength. When a-phase precipitation is assisted by the ω phase through heterogeneous nucleation, it occurs predominantly intragranularly, whereas ageing can also lead to intergranular precipitation at grain boundaries. Intragranular precipitation may also occur at low heating rates. This study investigated isothermal ω and α precipitation in the metastable Ti-19Nb-2.5Fe-6Sn (wt%) β alloy aged at 400 °C and 600 °C using transmission electron microscopy. An unusual absence of precipitation-free zones (PFZ) was observed at 400 °C without pre-ageing at a heating rate of 10 °C/min. This behaviour may be associated with higher oxygen levels or vacancy enrichment near grain boundaries after solution

treatment. Slower heating (5 °C/min) and pre-ageing at 300 °C increased the density of intragranular precipitates at both ageing temperatures. Lower chemical partitioning was observed after ageing at 300 °C for 9 h and increased after 12 h. Ellipsoidal precipitates were observed during pre-ageing and low-temperature ageing (400 °C), with depletion of Nb, Fe, and Sn. At 600 °C, α laths enriched in Sn were observed.

ME06 - The use of waste materials from the wood industry in the form of sawdust from pedunculate oak (Quercus robur) in processes for removing metals from the aquatic environment

Tomasz Kalak

Department of Industrial Products and Packaging Quality, Institute of Quality Science, Poznań University of Economics and Business, Poznań, Poland

Abstract

The contamination of aquatic systems with potentially toxic metals remains a significant environmental challenge, prompting the development of sustainable and cost-effective remediation methods. In this context, waste biomass from the wood industry represents a valuable source of low-cost biosorbents. This study addresses the potential application of pedunculate oak (Quercus robur) sawdust as an adsorptive material for the removal of metal ions from aqueous environments. As a lignocellulosic waste product, oak sawdust combines broad availability, low processing requirements, and biodegradability, which makes it particularly relevant to circular economy approaches in environmental engineering.

The sorption properties of Quercus robur sawdust are primarily associated with its heterogeneous porous structure and the presence of active functional groups, such as hydroxyl, carboxyl, and phenolic moieties, capable of interacting with metal ions via ion exchange, surface complexation, and physicochemical adsorption. The efficiency of the process is strongly influenced by operational variables, including pH, contact time, initial metal concentration, adsorbent dosage, and particle size distribution. Special attention is given to metals commonly occurring in industrial effluents.

Although raw oak sawdust generally exhibits lower adsorption performance than chemically modified sorbents, its environmental compatibility and economic advantages support its application as a promising biosorbent in preliminary or complementary wastewater treatment systems. Further investigation should focus on surface modification strategies, sorbent regeneration, adsorption kinetics and equilibrium modelling, and validation under real wastewater conditions.

ME07 - Improving the electrical response of metal oxide-based sensors.

Ricardo Henríquez1, Leonardo Vergara1, Valeria del Campo1, Rodrigo Segura2 and Douglas Olivares3.*

1 Universidad Técnica Federico Santa María, Chile; 2 Universidad de Valparaíso, Chile; 3 Universidad de Antofagasta, Chile.

Abstract

Sensors enhance human perception by detecting environmental stimuli and converting them into electrical signals. Among them, metal oxide thin-film sensors based on electrical response exhibit a wide range of applications [1]. This report presents a series of results aimed at improving the electrical performance of CuO-based sensors through morphological modifications introduced during the fabrication process. Copper thin films were deposited onto mica substrates using high-vacuum evaporation. The samples were subsequently oxidised in air for three hours at 300 °C. The deposition temperature of the copper films varied between room temperature (RT) and 300 °C. Additionally, in some samples, a 0.5 nm chromium layer was introduced as a surfactant [2]. SEM, Raman spectroscopy, and UV–Vis spectroscopy were performed on all samples. The characteristic CuO peak (296 cm^{-1}) was observed in all films, and the band gap was determined to be 1.78 eV using the Kubelka–Munk function as a function of photon energy [3]. The results indicate that increasing surface roughness enhances the electrical response by 10%, and the presence of a Cr surfactant layer enables a reduction in film thickness while maintaining comparable sensor performance.

Acknowledgement: This research was supported by Anid Fondecyt 1231849, Fondequip 190179, and EQM 220028.

[1] M. Yao et al., Frontiers in Chemistry 9, 608327.

[2] R. Henriquez et al., Applied Surface Science 489 (2019) 403–408.

[3] M. Khan et al., Nanomaterials 2020, 10, 1298.

ME08 - Structural and morphological tuning of CuO thin films for enhanced ethanol gas sensing

Leonardo Vergara 1, Ricardo Henríquez 1 Valeria del campo 1, Patricio Häberle 1, Rodrigo Segura 2*

1Universidad Técnica Federico Santa María, 2Universidad de Valparaíso

Abstract

Gas sensors are devices that detect changes in the environment and convert them into electrical signals. Thin copper films, 20 nm thick, have been fabricated in a high-vacuum thermal evaporation system on mica substrates. Growth parameters such as substrate temperature were modified. After deposition, the samples were oxidised in air at 300 °C for 3

h through an annealing process. Raman and UV-Vis spectroscopy were performed on all samples. The characteristic peak corresponding to CuO (296 cm-1) appears clearly. The Kubelka-Munk function, as a function of photon energy, yields a band gap of 1.78 eV. Temperature-dependent electrical resistance tests show semiconductor-like behaviour with an activation energy of 467 meV. The performance of the samples as a gas sensor was tested, measuring the electrical resistance of the films in the presence of ethanol gas at low pressure (from 10-3 to 103 Pa). Results show that the samples are sensitive and exhibit selectivity to ethanol gas.

The films were exposed to a controlled surface decoration process. Ultrathin chromium films with varying thicknesses (0.1–1 nm) were evaporated on copper oxide surfaces. The characteristic Cr2O3 peak (550 cm-1) appears in the films. Finally, the performance of the samples as gas sensors was tested again by measuring the electrical resistance of the films in the presence of low-pressure ethanol gas. Resistance changes of up to 50% were measured. The chromium layer exhibits an effect on this behaviour, which is discussed using a gas adsorption model in p-type semiconductors.

ME09 - Growth of ultrathin $NiCl_2$ films on Au(111) studied by STM

Javiera Martínez1, Patricio Häberle1, Juan Fernández2 y Ricardo Henriquez1*

1Universidad Técnica Federico Santa María, Chile, 2CIC nanoGUNE, San Sebastián, Spain

Abstract

Transition metal dihalides (TMDHs) are a class of two-dimensional (2D) layered materials bound by van der Waals interactions [1], which can be assembled layer by layer to achieve tunable electronic, mechanical, and thermal properties. Among these, the coexistence of magnetic ordering and semiconducting behaviour in the bulk form is particularly attractive, as it enables the development of spin-based microscopic devices.

In this work, we investigate the growth of nickel dichloride ($NiCl_2$) on Au(111), focusing on the key parameters governing film formation and thickness control. The objective is to obtain well-defined layers, including monolayers, bilayers, and thicker films.

Deposition rate, substrate temperature, and post-deposition annealing were systematically varied to identify optimal growth conditions. Experiments were carried out under ultra-high vacuum (UHV) conditions using a system equipped with a deposition source, a thickness monitor, and a scanning tunnelling microscope (STM). The structural and electronic properties of the resulting films were characterised by STM, with particular emphasis on surface topography as a tool to optimise growth protocols.

[1] K. S. Novoselov, A. Mishchenko, A. Carvalho, and A. H. Castro Neto, 2D Materials and van Der Waals Heterostructures, Science (1979) 353, (2016)

ME10 - Spintronic potential of Co/Cr_2O_3 interfaces: oxidation and exchange bias effects

Fernando Alvarez-Asencio1,2, Ricardo Henríquez1*

1Universidad Técnica Federico Santa María, Chile, 2Pontificia Universidad Católica de Valparaíso, Chile

Abstract

As CMOS-based electronic scaling approaches its fundamental physical limits, spintronics emerges as a compelling alternative to conventional semiconductor paradigms. This study investigates the electrical, magnetic, and optical properties of cobalt (Co) thin films as the ferromagnetic (FM) component, focusing on functional degradation induced by oxidation. Utilising high vacuum (HV) physical vapour deposition (PVD), Co films (1–10 nm) were synthesised to evaluate the evolution of their transport properties under controlled oxidation. To mitigate this degradation, a chromium (Cr) passivation layer was introduced, where the resulting chromium oxide (Cr_2O_3) acts as an antiferromagnetic (AFM) layer. The results indicate that oxidation kinetics follow a layer-by-layer growth mechanism consistent with Cabrera–Mott theory [1], with Co reaching saturation at higher air pressures compared to Cr. This differential kinetic behaviour enables precise control of the oxidation flux within the Co/Cr_2O_3 bilayer, optimising the stability of the ferromagnetic phase. Moreover, the FM/AFM interface exhibits exchange bias effects [2], providing enhanced magnetic anisotropy and stability crucial for spintronic applications. Finally, the incorporation of a gold (Au) capping layer is proposed to establish an FM/AFM/NM trilayer architecture. In this system, Au serves a dual role: acting as a chemical passivation barrier and, leveraging its strong spin–orbit coupling [3], functioning as a strategic component for spin current manipulation and spin–orbit torque phenomena.

[X] Cabrera, N., & Mott, N. F. (1949). Theory of the oxidation of metals. Reports on Progress in Physics, 12, 163–184. https://doi.org/10.1088/0034-4885/12/1/308

[Y] Nogués, J., & Schuller, I. K. (1999). Exchange bias. Journal of Magnetism and Magnetic Materials, 192(2), 203–232. https://doi.org/10.1016/S0304-8853(98)00266-2

[Z] Kent, A. D., & Worledge, D. C. (2015). A new spin on magnetic memories. Nature

Nanotechnology, 10(3), 187–191.
https://doi.org/10.1038/nnano.2015.24https://doi.org/10.1103/PhysRev.102.1413

ME11 - Microstructural Evolution and Phase Transformation Pathways in Metastable

β-Ti Alloys produced by EB-PBF

Matheus Valentim1

**, Rubens Caram1*

School of Mechanical Engineering – University of Campinas (UNICAMP), Brazil

Abstract

Metastable β-titanium alloys produced by additive manufacturing exhibit complex microstructural evolution due to rapid solidification, strong crystallographic texture, and subsequent thermally activated phase transformations. Understanding the mechanisms governing the formation and evolution of secondary phases is essential to control the mechanical behaviour of these alloys, particularly for structural and biomedical lattice applications. In this work, the microstructural evolution of additively manufactured metastable β-Ti alloys is investigated using advanced electron microscopy techniques combined with crystallographic analysis. Electron backscatter diffraction (EBSD) was employed to characterise grain morphology, crystallographic texture, and local misorientation metrics such as Kernel Average Misorientation (KAM) and Grain Orientation Spread (GOS), providing insights into deformation and stored energy distribution. Transmission electron microscopy (TEM) and scanning transmission electron microscopy (STEM) analyses were conducted to identify nanoscale phase transformations and orientation relationships between the β matrix and transformation products. Special attention is given to the nucleation and growth of the hexagonal phase during thermal exposure, as well as to variant selection mechanisms associated with crystallographic orientation relationships. The influence of strong solidification textures typical of additive manufacturing on phase transformation pathways is discussed. Additionally, diffraction-based analysis and orientation mapping approaches are used to correlate phase morphology with crystallographic constraints. The results provide insights into the transformation mechanisms operating in metastable β-Ti alloys and their relationship with local crystallography and thermal history. These findings contribute to the understanding of microstructure–property relationships in additively manufactured titanium alloys and support the design of architected materials with tailored mechanical performance.

ME12 - Controlled Electrochemical Surface Nanostructuring of Metallic Glasses: A Platform for Tailored Functional Properties

Viktoriia Shtefan1,2, Annett Gebert1*

1Leibniz Institute for Solid State and Materials Research Dresden, Germany; 2National Technical University "Kharkiv Polytechnic Institute", Ukraine

Abstract

The surface engineering of metallic glass alloys allows for the creation of highly functional interfaces thanks to their chemical homogeneity, structural isotropy and tunable electronic structure. This study presents a controlled electrochemical nanostructuring approach for two multicomponent metallic glass systems, involving selective anodic oxidation and dealloying in non-toxic electrolytes.

The first system, a Ti-Cu-Zr-based bulk metallic glass, was anodised in a potassium pyrophosphate electrolyte at room temperature. This formed a bilayered oxide film

containing a dense, amorphous inner layer (7–10 nm) and a porous outer layer (15–75 nm) with uniformly distributed copper nanocrystals. Advanced characterisation reveals that the nanocrystals formed via complexation-driven copper mobilisation, followed by partial reduction within the oxide matrix. The resulting surface architecture exhibits improved stability in chloride-containing environments with suppressed localised degradation.

The second system, a Zr-Ni-based metallic glass, was investigated as a precursor for the development of a nanoporous surface via selective electrochemical dealloying. Controlled pulsed etching creates a three-dimensional porous network with tunable ligament and pore dimensions; the composition of the precursor governs the distribution of low-coordination sites and surface chemistry.

Comparative electrochemical analysis shows that this nanostructuring approach improves surface passivation, charge transfer characteristics and long-term operational stability consistently across both alloy families. This methodology provides a rational framework for designing advanced functional surfaces. Current research is extending this approach towards green energy conversion technologies, including hydrogen evolution reactions.

V. Shtefan thanks the Deutsche Forschungsgemeinschaft (DFG) for funding this work under project no. 458057521 (GE 1106/15-1) and no. 553576450 (SH 2178/1-1).

ME13 - Constitutional Supercooling Strategies for Additive Manufacturing Grain

Refinement: Effect of increasing Cu additions in the Ti-42Nb Alloy

Hugo Magalhães1, Carlos da Silva[1], Matheus Valentim[1], Gilberto Prandi[1], João Rodrigues[1], Kaio Niitsu[1], Rubens Caram[1]*

[1]State University of Campinas, Brazil

Abstract

Metastable β-Ti alloys, such as Ti-42Nb, combine low elastic modulus with excellent biocompatibility, making them attractive for the fabrication of biomedical implants via Laser Powder Bed Fusion (LPBF).

Nevertheless, their performance is often compromised by strong mechanical anisotropy arising from coarse columnar grains formed during solidification. The addition of alloying elements can effectively overcome this limitation by enhancing solute partitioning and amplifying constitutional supercooling (CS),stimulating grain refinement. These elements are selected for their growth restriction factor (Q), widening the solidification range (ΔT) and forcing a columnar-to-equiaxed transition (CET), reducing both grain size and anisotropy.

CALPHAD simulations predicted a high capacity for Cu-induced CS. These predictions were validated by arc-melted Ti-42Nb-xCu (x=1~5 wt.%) samples, which displayed both finer dendrites and higher hardness due to microstructure refinement and precipitate formation. Then, LPBF produced dense (>99%) samples with varying Cu contents (0, 1, 5 and 10 wt.%).

Low Cu (1 wt.%) yielded finer cells and minimal cracking, 5 wt.%Cu promoted CET but also peak hot tearing due to an extensive interdendritic Ti2Cu network, and 10 wt.%Cu reduced crack formation while promoting maximum grain refinement.

This trend mirrors classic hot cracking behaviour: minor Cu forms a thin terminal film not capable of backfilling grain boundary tears, whereas higher Cu boosts eutectic volume, which quickly fills gaps via liquid backflow. Cu addition also disrupted the preferential <001>//BD texture (MRD≈1), successfully promoting equiaxed grains via CS driven nucleation. These findings help define optimal parameters for achieving crack-free and isotropic LPBF parts with improved long-term performance.

ME14 - Development of Poly(4-vinylpyridine)-Wrapped Carbon Nanotubes with Metal Nanoparticle Decoration for High-Sensitivity Hydrogen Detection

Presenter* and Co-author names {Andrea Gonzalez Minaya[1]*, Prof. Dr. Máté Bezdek[1], Prof. Dr. Timothy M. Swager[2], Thomas Pioch[1].}

Affiliation {[1]ETH Zurich (Eidgenössische Technische Hochschule Zürich), Switzerland;

[2]Massachusetts Institute of Technology (MIT), USA.}

Abstract

Reliable hydrogen detection is essential for the safety of emerging green energy infrastructures. While carbon nanotube-based chemiresistors offer a promising platform for gas sensing, achieving the sensitivity and long-term stability required for practical applications remains a challenge. In this work, surface-anchored carbon nanotubes wrapped in poly(4-vinylpyridine) (P4VP) were decorated with metal nanoparticles via electron-beam deposition to investigate their performance as hydrogen sensors. Investigated configurations included palladium, platinum, and combinations with additional copper and cobalt. Experimental results demonstrated robust response magnitudes of approximately 15% at 5000 ppm, with detectable signals maintained at concentrations as low as 300 ppm. A key finding was the role of the polymer-carbon nanotube interaction: while P4VP wrapping initially induced n-type doping, subsequent chemical quaternization successfully reverted the network to p-type behaviour, enabling control over the doping state. Additionally, baseline resistance was identified as a critical parameter, with a mid-kΩ range found to be optimal for signal-to-noise ratios. The highest performance was achieved by quaternized palladium and platinum nanoparticle sensors, which exhibited a measured experimental limit of detection (LOD) of 300 ppm. These results demonstrate that interfacial doping control through polymer quaternization is a highly effective strategy for enhancing the performance of carbon-nanotube-based hydrogen sensors.

ME15 - Bridging Data Science and Battery Engineering: Analytical Equations for LMB Capacity Retention via Machine Learning and Symbolic Regression

Hyo-Jin Joo1,2, In-Ho Choi1,2, Dong-Hwa Jung1, Min-Ho Kang1,2,3**

1Department of Biomedical-Chemical Engineering, The Catholic University of Korea, Bucheon-si, Gyeonggi-do, Republic of Korea

2Department of Biotechnology, The Catholic University of Korea, Bucheon-si, Gyeonggi-do, Republic of Korea

3Research Institute for Controlled Biomaterials of Regulated Cell Death, The Catholic University of Korea

Abstract

Lithium metal batteries (LMBs) are widely regarded as promising candidates for next-generation, high-energy-density storage devices capable of surpassing conventional lithium-ion technology. However, their practical commercial application remains severely limited due to rapid electrochemical degradation. This degradation is primarily driven by uncontrolled lithium dendrite growth and continuous electrolyte depletion during repeated cycling, which compromises both safety and long-term stability. While artificial intelligence and machine learning have increasingly aided in battery performance prediction, existing "black-box" models present a significant limitation: they often lack the fundamental interpretability required for rational material optimisation. To overcome this challenge, this study proposes a robust, data□driven approach to derive a transparent, closed-form mathematical expression for predicting the capacity retention of NCM-based LMBs. We systematically constructed a comprehensive dataset comprising 14 critical design variables, including detailed electrolyte composition, varying NCM stoichiometry, and specific cathode loading parameters. By innovatively integrating feature importance analysis with advanced symbolic regression techniques, we successfully identified the dominant factors determining cycle life and formalized them into highly interpretable equations. Unlike opaque existing models, our derived mathematical equations clearly elucidate the complex, nonlinear correlations between electrolyte formulations and overall electrochemical performance. Ultimately, this approach provides practical descriptors for optimizing cell composition, significantly accelerating battery design and effectively bridging the gap between advanced data science and fundamental battery engineering.

ME16 - Surface Engineering of Si@void@C Yolk–Shell Anode via GQD Coating for Superior Capacity Retention in Li-Ion Batteries

*JiHye Kim1,2, Min-Ho Kang1,2,3**

1Department of BioMedical-Chemical Engineering, The Catholic University of Korea, Korea;

2Department of Biotechnology, The Catholic University of Korea, Korea;

3Research Institute for Controlled Biomaterials of Regulated Cell Death, The Catholic University of Korea

Abstract

Silicon (Si) anodes possess an exceptionally high theoretical capacity; however, their practical implementation is severely hindered by substantial volume expansion and rapid capacity fading during repeated lithiation and delithiation processes. To address these intrinsic challenges, a yolk–shell structured Si anode with a controlled internal void space was rationally designed to effectively accommodate volumetric expansion while preserving structural integrity. To further enhance electrochemical performance, graphene quantum dots (GQDs) were uniformly decorated onto the surface of the yolk–shell structure. As zero-dimensional graphene-based nanomaterials, GQDs exhibit high electrical conductivity and facilitate the formation of efficient electron transport networks across the electrode. The introduction of GQDs markedly improved the overall electrical conductivity, which consequently led to enhanced capacity retention and prolonged cycling stability compared to the pristine yolk–shell Si anode. The synergistic integration of structural buffering and surface conductivity enhancement effectively mitigates the fundamental limitations of Si-based anodes. This integrated design strategy provides a promising approach for the development of high-performance and durable silicon anodes for advanced lithium-ion battery applications.

ME17 - Nanosized Silicon Confined in 3D Porous MoS2 Frames for High Capacity and Cycling Stability in Lithium-Ion Battery

Inho Choi1,2,, Min-Ho Kang1,2,3**

1The Catholic University of Korea; Department of Biomedical-Chemical Engineering, Korea

2The Catholic University of Korea; Department of Biotechnology, Korea

3The Catholic University of Korea; Research Institute for Controlled Biomaterials of Regulated Cell Death, Korea

Abstract

Nanosized silicon (Si) confined in 3D porous MoS2 frames were synthesized via a salt-template□assisted thermal synthesis combined with a vacuum-driven Si nanoparticle (SiNP) infiltration method to achieve high-performance lithium-ion battery anodes. The robust, interconnected 3D porous MoS_2 framework suppresses restacking of MoS2 2D layers and establishes porous pathways that accelerate Li ion and electron transport. The composite exhibits a capacity exceeding the theoretical limit of MoS_2 (670 mAh g^{-1}) through synergistic effects arising from the high surface area of the porous architecture of MoS2 and the superior theoretical capacity of Si. In addition, volume expansion and pulverisation of Si during cycling are suppressed due to the confinement effect of porous MoS2 frameworks. Consequently, the initial irreversible capacity is mitigated by suppressing additional SEI

formation and Li trapping within the Si. The unique 3D porous framework structure further improves mechanical integrity and cycling stability. Collectively, these results identify the SiNP-confined 3D porous MoS_2 composite as a promising anode material for advanced lithium-ion batteries with high capacity and long-term cycling stability.

ME18 - Uniform Carbon-Coated SiOX anodes via PDDA-Assisted RF Gel Assembly and Magnesiothermic Reduction

*Eunsaem Song1, Min-Ho Kang1,2,3*1*

1Department of BioMedical-Chemical Engineering, The Catholic University of Korea, Korea;

2Department of Biotechnology, The Catholic University of Korea, Korea; 3Research Institute for

Controlled Biomaterials of Regulated Cell Death, The Catholic University of Korea

Abstract

This study introduces a novel strategy for fabricating uniform carbon-coated SiOx nanostructures with internal void spaces to enhance the electrochemical performance of lithium-ion battery anodes. To ensure high structural uniformity, monodisperse silica spheres were first modified with poly(diallyldimethylammonium chloride) (PDDA), a cationic polymer, to create a positively charged surface. This surface modification enabled the precise electrostatic assembly of resorcinol-formaldehyde (RF) gel, resulting in a highly uniform coating layer. The obtained carbon-coated SiO2 was subsequently subjected to a controlled magnesiothermic reduction process to partially reduce the core into SiOx. This approach offers two critical advantages: first, the SiOx core significantly improves the theoretical capacity compared to pristine silica; second, the deliberate incorporation of internal void structures effectively accommodates the large volume expansion of silicon during lithiation, preventing mechanical pulverisation and ensuring long-term structural stability. The resulting uniform carbon layer further enhances electrical conductivity and promotes the formation of a stable solid-electrolyte interphase (SEI). This synthesis method provides a scalable and efficient pathway for developing high-performance, durable silicon-based anode materials.

ME19 - Molybdenum Disulfide for Battery Applications

*Hae Kyung Jeong **

Department of Energy and Battery Engineering, Daegu University, Republic of Korea

Abstract

Molybdenum disulfide (MoS_2) is synthesised and modified for battery applications. It shows various morphologies and dimensions depending on the conditions and processes of the

synthesis. The synthesised molybdenum disulfide is carefully characterised by using XRD, SEM, Raman spectroscopy, and XPS. In addition, its electrochemical properties are also investigated by using a potentiostat and galvanostat with electrochemical impedance spectroscopy for battery applications. Cyclic voltammetry, Galvanostatic charging and discharging measurements are performed. In addition, electrochemical impedance is also measured from 1 mHz to 1 kHz. The results might evaluate whether MoS_2 could be used as an anode material, instead of carbon material, especially graphite, for battery applications.

ME20 - Core-Controlled Assembly Mechanisms of Virus-Like Particles

Monica Enculescu1,2, Anca Aldea1,2, Maria-Lorena Jinga1,2, Irina Tsvetkova2,3, and Bogdan Dragnea2,3*

1National Institute of Materials Physics (NIMP), Magurele, 077125, Romania

2International Center for Advanced Training and Research in Physics (CIFRA), Magurele, Romania

3Department of Chemistry, Indiana University, Bloomington, IN 47405, USA

Abstract

Virus-like particles (VLPs) are widely used in drug delivery and vaccine development. Assembling VLPs in vitro is used for studying the thermodynamics and kinetics of the assembling processes. Brome mosaic virus (BMV) is one of the simplest and most thoroughly studied plant viruses. The capsid of BMV is composed of 180 identical protein molecules which are clustered into hexamers and pentamers on the surface. The capsid's diameter is about 28 nm and has an 18 nm inner cavity. These capsids can be used for specific and localised treatment; therefore, it is important to study the thermodynamics of their assembling processes. Thus, gold nanoparticles (GNP) with diameters that can be controlled from the synthesis were used as a cargo model.

For incorporation of gold nanoparticles into the viral capsid, the GNPs were functionalized with specific ligands which contain a hydrophobic alkaline chain with a thiol group on one side and a polyethene glycol chain with a carboxylic group on the other, ensuring the requirements for an assembly promoter: a negative surface charge for interaction with viral proteins, flexibility and hydrophilicity. The size of the gold particle has an influence on the structure of the resulting VLP and alters the yield of VLP emission. This study proposes the investigation of the influence of the GNP size on the icosahedral configurations of the VLPs and on the assembly mechanisms. For that, GNPs with different diameter values were used in fluorescence titration experiments to determine each phase in the assembly process.

Acknowledgements

The authors thank the National Authority for Scientific Research through project PNRR Ctr. 760099/23.05.2023.

ME21 - Developed a multifunctional local drug delivery system based on zinc-magnesium layered hydroxide nanoparticles (Zn–Mg LH NPs) loaded with doxycycline

*Victor Martin1,2, Maria Helena Fernandes1,2, Ana Francisca Bettencourt3, Pedro Sousa Gomes1,2, Catarina F. Santos3, 4,5**

1 – BoneLab, Faculdade de Medicina Dentária, Universidade do Porto, Rua Dr. Manuel Pereira da Silva, 4200-393 Porto, Portugal.

2 - LAQV/REQUIMTE, Faculdade de Medicina Dentária, Universidade do Porto, Rua Dr. Manuel Pereira da Silva, 4200-393 Porto, Portugal.

3 – Research Institute for Medicines (iMed.ULisboa), Faculty of Pharmacy, Universidade de Lisboa, Avenida Prof. Gama Pinto, 1649-003 Lisboa, Portugal.

4 – CQE, IMS, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal.

5 - EST Setúbal, Instituto Politécnico de Setúbal, Campus IPS, 2910 Setúbal, Portugal.

Abstract

Periodontitis is a chronic inflammatory disease resulting in the progressive destruction of tooth-supporting tissues, largely driven by dysbiotic subgingival biofilms [1]. Current treatments rely on mechanical debridement complemented by systemic or local antimicrobials, which suffer from limited subgingival effectiveness and undesirable side effects. To overcome these drawbacks, this study developed a multifunctional local drug delivery system based on zinc-magnesium layered hydroxide nanoparticles (Zn–Mg LH NPs) loaded with doxycycline (DX). The nanoparticles were synthesised via a single-step co-precipitation route. Transmission electron microscopy revealed nanoscale lamellar morphologies, with mean dimensions below 100 nm, while selected-area electron diffraction and X-ray diffraction confirmed the formation of Zn-Mg layered hydroxide phases. The incorporation of doxycycline modified the crystallinity and morphology, producing smaller, more dispersed particles and partial structural amorphisation indicative of intercalation within the hydroxide layers. FTIR analysis confirmed characteristic Zn–OH vibrations and distinct doxycycline bands, demonstrating successful drug incorporation. Zeta potential analysis showed a strong positive surface charge (> +30 mV) for unloaded NPs, decreasing with increasing drug content, consistent with surface adsorption of anionic doxycycline species. Inductively coupled plasma spectroscopy revealed reduced Zn^{2+} release upon drug incorporation, suggesting partial ion substitution. The DX5-Zn-Mg formulation displayed high encapsulation efficiency and a sustained release profile, releasing 50% of the drug at neutral pH and 100% under acidic conditions, ideal for targeting the inflamed periodontal microenvironment. Biologically, DX5-Zn-Mg NPs exhibited strong antioxidant and antibacterial activity, biocompatibility with human gingival fibroblasts and significant downregulation of pro-inflammatory genes (IL1B, IL6, CXCL8, NFκB) in a 3D oral mucosa

model. Altogether, doxycycline-loaded Zn–Mg LH NPs represent a stable, bioactive, and locally effective therapeutic platform for the treatment of periodontitis.

ME22 - Nanosystems Encapsulating Essential Oils of Aromatic Plants for the Control of Tetranychus Urticae and Tuta Absoluta

Ioanna Pitterou[1], Anna Karantoni[1], Zacharoula Zampeti[1], Aikaterini Barouni[1], Sofia Vichou[1], Sofia Dervisoglou[2], Theodoros Stathakis[2], Evangelos Fytas[2], Dionysios Perdikis[2], Anastasia Detsi[1]*

[1]*Laboratory of Organic Chemistry, School of Chemical Engineering, National Technical University of Athens, Greece*

[2]*Laboratory of Agricultural Zoology & Entomology, Department of Crop Science, School of Plant Sciences, Agricultural University of Athens, Greece*

Abstract

Essential oils (EOs) derived from aromatic plants have shown promising potential in the control of agricultural pests. Moreover, their encapsulation in biodegradable and biocompatible nanosystem carriers may enhance their stability, controlled release, and overall bioactivity. In this study, the essential oils of four aromatic plants—lavender (*Lavandula officinalis*), laurel (*Laurus nobilis*), cardamom (*Elettaria cardamomum*), and clove (*Syzygium aromaticum*)—were encapsulated in yeast cells, chitosan, and β-cyclodextrin (β-CD) and evaluated for their pesticidal potential. More specifically, the toxicity and repellent effects of these EO nanoformulations were assessed against nymphs and adults of the two-spotted spider mite, *Tetranychus urticae* Koch (Acari: Tetranychidae). In addition, their ovicidal activity was evaluated against eggs of the tomato pinworm, *Tuta absoluta* Meyrick (Lepidoptera: Gelechiidae) on tomato leaflets. The chemical composition of each essential oil was determined using gas chromatography–mass spectrometry (GC–MS).

Acknowledgement

This work has been produced with the financial assistance of the European Union under the Interreg NEXT MED Programme within the framework of Project No. A_T_1.1_0167-EONANOBIOPS ‘Essential Oil-derived Next Generation Nano-Biopesticides for Sustainable Eco-Friendly Agriculture’.

ME23 - Design Of an Actuator for Linear Displacement by Shape Memory Alloy

Pan chi hsiang

National Chin-Yi university of technology, Taiwan (R.O.C)

Abstract:

Conventional machines or robots use traditional hydraulic, pneumatic, or electric motor actuators for displacement operations. However, shape memory alloy (SMA) actuators can simplify the complexity, size, and weight of machine or robot components, as well as reduce noise generation. In this paper, a new actuating mechanism driven by shape memory alloy (SMA) with linear displacement has been designed and implemented. First, the helical spring-shaped SMA element is fabricated from SMA wire with a one-way shape memory effect. Subsequently, the actuating mechanism for linear displacement driven by the helical spring-shaped SMA element is developed. The actuating mechanism is driven by heating (or electrical heating). Although the response time (or actuation time) is slower than that of traditional actuators and the displacement accuracy is not high, it has some advantages: (1) compact, lightweight and easy to miniaturise; (2) adjustable to modify the performance of the mechanism; (3) it is easily to assemble and disassemble. The performances of the bending actuating mechanism, such as the response time (rise and recovery in an actuating cycle) and the displacement in terms of the driving currents, are evaluated through the experiment. The actuating mechanism provides a high possibility of application for its large displacement, high power-to-weight ratio, easy for miniaturization, quiet operation, suitability for cleanliness requirements, and lower cost than conventional actuators.

ME24 - Martensitic transformation influence on crack behaviour in beta metastable Ti-5553 alloy.

C. S. A. da Silva1, H. M. de Azevedo1, M. Valentim1, G. V. Prandi1, J. F. Q. Rodrigues1, M. Sangali1, L. A. Leão2, R. Caram1.*

1School of Mechanical Engineering, University of Campinas, Brazil.

2School of Applied Sciences, University of Campinas, Campinas, Brazil.

Abstract

The martensitic transformation is an intriguing phenomenon that can either enhance or degrade the properties of metallic materials containing metastable phases. In this context, titanium alloys with a BCC structure—specifically, the beta metastable titanium alloys—are of particular interest. Most beta metastable titanium alloys exhibit extensive plastic deformation mechanisms, which can be primarily attributed to the effects of Twinning-Induced Plasticity (TWIP) and Transformation-Induced Plasticity (TRIP). These phenomena arise due to the limited strain-hardening capability of BCC-structured titanium alloys. One notable example is the commercially significant Ti-5553 alloy, which stands out as a promising material for investigating the dominant plastic deformation mechanisms in

metastable titanium alloys. Numerous studies have focused on analysing twinning systems, particularly the {112} and {332} or other twinning systems modes in BCC titanium alloys. Additionally, the Stress-Induced Martensitic Transformation (SIMT) from BCC to orthorhombic or BCC to omega phases has been widely reported to influence the mechanical response. Furthermore, some studies have demonstrated that the SIMT mechanism can also be utilised for grain refinement, thereby enhancing mechanical strength. However, other research has highlighted important insights regarding of fracture behaviour associated with the SIMT mechanism. To support our discussion, results from Scanning Electron Microscopy (SEM), Electron Backscatter Diffraction (EBSD), and Transmission Electron Microscopy (TEM) will be presented and analysed.

ME25 - Laser-Assisted Nanostructured rGO/PVA Polymer Materials for Energy Applications

Maha Al-Hamadani and Haitham Al-Tameemi*

*Department of Physics, College of Science, University of Basrah, Basrah, Iraq**

Abstract

We developed laser-assisted nanostructured polymer materials from poly(vinyl alcohol) (PVA) reinforced with reduced graphene oxide (rGO) and conducted a thorough investigation of their energy-related applications. We fabricated rGO/PVA nanocomposite films via a controlled solution-casting technique to ensure uniform distribution of rGO nanosheets inside the polymer matrix. We selected reduced graphene oxide as an active nanofiller due to its superior electrical conductivity, extensive surface area, and exceptional light absorption capacity. These are essential attributes for materials used for energy storage.

Continuous-wave laser stimulation in the visible spectral region was employed as an external stimulus to enhance light–matter interaction and induce optical alterations in the nanostructured polymer system. Experimental results indicate that laser-assisted contact significantly enhances optical absorption compared to pure PVA sheets. The rGO/PVAnanocomposites exhibit an absorption enhancement factor of around 3 to 5 times, contingent upon the concentration of rGO and the intensity of the laser. A corresponding reduction in optical transmission above 30–40% was observed, indicating improved energy absorption capability suitable for optically active energy materials.

The impact of rGO concentration on material performance was meticulously analyzed. The optimal loading range was determined to be around 0.5–1.0 wt% rGO, which provides the most effective optical improvement while maintaining film uniformity and stability. Increased levels of rGO lead to significant aggregation effects, perhaps resulting in saturation or a little reduction in optical sensitivity. The identified patterns are attributed to nanoscale dispersion, an increased surface-to-volume ratio, and laser-induced charge redistribution at the rGO/PVA interface.

The findings indicate that rGO/PVA nanostructured polymer materials fabricated using lasers are suitable for energy-related applications.

ME26 - Scalable FAST/SPS Processing of TiNbTaHfMo High-Entropy Alloys for Biomedical Implants: Linking Microstructure to Mechanical and Corrosion Performance

Sheila Lascano1, Cristina Arévalo2, Fabián Sánchez-Parrines1, Ricardo Chávez-Vásconez1, Karina Muñoz-Becerra3, Ricardo Venegas3, Dana Gentil1, Yadir Torres2*

1Universidad Técnica Federico Santa María, Chile; 2Universidad de Sevilla, España; 3Facultad de Ciencias de la Salud, Universidad Bernardo O´Higgins, Chile.

Abstract

The increasing demand for advanced orthopaedic implants requires biomaterials with reduced elastic modulus, enhanced corrosion resistance, and improved osseointegration. Conventional alloys such as Ti□6Al-4V and Co–Cr systems often exhibit mechanical mismatch with bone tissue and potential ion release, leading to stress shielding and long-term implant failure. High-entropy alloys (HEAs) composed of biocompatible elements have emerged as promising candidates for next-generation biomedical applications.

In this work, a $Ti_{30}Nb_{25}Ta_{25}Hf_{10}Mo_{10}$ (at.%) HEA was designed using thermodynamic and electronic parameters ($\Delta S_{mix} \approx 1.51R$, $\delta \approx 3.14\%$, VEC ≈ 4.7), predicting the formation of a BCC solid solution with reduced stiffness. Porous structures were fabricated through a scalable powder metallurgy route combining a space-holder technique with FAST/SPS processing. Elemental powders were mixed with 0–60 vol.% ammonium carbonate to control porosity, followed by sintering at 1450 °C for 10 min. Microstructural characterisation revealed partial elemental diffusion and heterogeneous regions, indicating ongoing homogenization during SPS. Porosity increased with spacer content, producing interconnected pore structures within the range suitable for bone ingrowth (~100–500 μm). Mechanical characterisation via micro- and nano-indentation showed consistent hardness trends, confirming the structural integrity of the porous network. Accelerated electrochemical analysis performed in a simulated physiological medium demonstrated favourable corrosion resistance, attributed to the formation of stable passive oxide layers associated with Ti-, Nb-, and Ta-rich regions.

These results highlight the potential of porous TiNbTaHfMo HEAs for load-bearing biomedical implants. Furthermore, FAST/SPS processing is demonstrated as a viable and scalable route for tailoring structure–property relationships in next-generation metallic biomaterials.

ME27 - Development of novel, stable, efficient and unclonable nanoscale luminescent ink for advanced anti-counterfeiting applications

Payal P. Pradhan, D. Haranath*

Luminescent Materials and Devices (LMD) Group, Department of Physics, National Institute of Technology Warangal, Hanumakonda - 506004, Telangana, INDIA.

Abstract

Counterfeiting remains a serious challenge for securing confidential documents and currency, driving the search for new materials with reliable optical signatures. In this work, we present a $Y_2SrZnO_5:Eu^{3+}$(YSZO: Eu^{3+}) nanopowder synthesised through a carefully optimised sol–gel combustion process. The phase purity, crystal structure, and lattice parameters were characterised by powder XRD and TEM analyses. FESEM confirms the surface morphology with a uniform size distribution at ~200 nm. YSZO: Eu^{3+} produces a vivid red emission between 550 and 700 nm, corresponding to the $^5D_0 \rightarrow {}^7FJ$ (J = 0–3) transitions of Eu^{3+}, with a measured colour purity of 99.8%. It has a greater External QY of 87%, 41% and 56% at 254, 393 and 465 nm, respectively. A novel PVA/oleic acid -based transparent ink medium was designed to serve as a host matrix for security ink formulations. Fourier transform infrared (FTIR) spectroscopy confirmed the compositional characteristics of the ink medium. When Nanopowders are formulated as an ink, it allows security patterns to remain invisible under daylight yet glow sharply under UV (254 nm), near-UV (393 nm), or blue (465 nm) illumination. The resulting security ink demonstrates remarkable photostability under 254 nm UV light, withstands heating up to 120 °C, and maintains its luminescent performance even after exposure to solvents and humid environments. Its robustness in different environments supports sustained stability, making it highly suitable for security and authentication uses. In contrast to conventional luminescent inks that rely on toxic solvents, this water-based system offers a safe, sustainable, and highly selective alternative. These combined properties establish YSZO: Eu^{3+} as a strong candidate for next-generation secure printing and currency protection.

ME28 - Laser-Based Nanostructured Photonic Polymer Sensors Based on ZnO/PMMA Nanocomposites

Haitham Al-Tameemi

Department of Physics, College of Science, University of Basrah, Basrah, Iraq

Abstract

Nanostructured materials were employed in the development and experimental evaluation of laser□based photonic polymer sensors to enhance optical sensing performance. This study employed poly(methyl methacrylate) (PMMA) as a transparent polymer matrix and included zinc oxide (ZnO) nanoparticles as optically active nanofillers to fabricate ZnO/PMMA nanocomposite sensing films. The nanocomposites were fabricated using a fluid casting

technique that facilitated regulated nanoparticle distribution. Subsequently, they were evaluated using a 532 nm visible laser.

We evaluated the sensor's responsiveness by employing lasers to alter the optical transmission and effective refractive index. The ZnO/PMMA nanocomposite sensors exhibited a much superior photonic response compared to pristine PMMA films. The optical signal amplitude rose by more than one order of magnitude under consistent laser excitation conditions, indicating an enhancement in the sensor's sensitivity. This enhancement results from intensified interactions between light and matter, increased scattering at the interface, and significant alterations in the refractive index induced by uniformly dispersed nanoscale surfaces.

We examined laser-induced photothermal effects, which yielded consistent, repeatable sensor readings with strong linearity across the spectrum of optical power analysed. The sensors exhibited negligible signal drift throughout several measurement cycles, indicating their stability and reliability. Furthermore, careful variation of ZnO nanoparticle concentration established an optimal loading range that improved optical sensitivity while preserving enough transparency for photonic detection.

To validate the experimental results, analysis and Density Functional Theory calculations were performed to investigate charge transport and alterations in the electronic structure at the ZnO/PMMA interface. The results indicate that the interaction between the two surfaces has intensified and the charge has redistributed, corroborating findings from tests that demonstrated an enhancement in optical transmission efficiency.

ME29 - Microstructural characterization of Ti-6Al-4V-xCu alloys

Tamara Holjevac Grgurić1, Primož Mrvar2, Mitja Petrić2, Stevica, Hodić3, Vilko Mandić4, Lucija Lasić1 and Karla Knežević1*

1Catholic University of Croatia, Technical Faculty, Ilica 244, 10000 Zagreb, Croatia

2Faculty of Natural Science and Engineering, University of Ljubljana, Aškerčeva cesta 12, Ljubljana, Slovenia

3Instrumentaria d.d., Rimski put 31, Sesvete, Croatia

4University of Zagreb, Faculty of Chemical Engineering and Technology, Marulićev trg 19, 10000 Zagreb, Croatia

Abstract

Copper-containing Ti-6Al-4V alloys have attracted interest in biomedical applications because they may combine excellent mechanical performance with intrinsic antibacterial properties. This study systematically investigated the microstructure, phase composition, thermal behaviour, and mechanical properties of a Ti-6Al-4V-Cu alloy to evaluate its suitability for implant applications.

The alloy was prepared by melting in an electric-arc furnace and cast into cylindrical ingots with different copper contents. The specimens were characterised using scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM-EDS), X-ray diffraction (XRD), differential scanning calorimetry (DSC), and Vickers microhardness testing. SEM-EDS analysis and XRD confirmed the formation of the intermetallic Ti_2Cu phase in addition to the α/β titanium matrix. The presence of Ti_2Cu is of particular importance, as this phase is associated with enhanced antibacterial performance and precipitation strengthening. DSC analysis provided insight into the thermal behaviour of the alloy and supported the occurrence of phase transformations related to the Cu-containing microstructure.

Microhardness measurements showed a significant increase relative to the conventional Ti-6Al-4V alloy, indicating that Cu addition and Ti_2Cu precipitation effectively strengthen the material. The improved hardness is expected to enhance wear resistance, a desirable property for long-term orthopaedic implant performance.

The combined microstructural, phase, thermal, and mechanical characterisation demonstrates that the Ti-6Al-4V-Cu alloy exhibits promising properties for biomedical applications. The formation of the Ti_2Cu intermetallic phase and the significant increase in microhardness suggest that this alloy represents a viable candidate for the development of next-generation orthopaedic implants with improved mechanical performance and potential antibacterial functionality.

DAY – 3, ROOM - A

Invited Talk

Biopolymers and Essential Oils: a Perfect Combination for the Development of Biocompatible Nanosystems and Materials

Anastasia Detsi, Ioanna Pitterou, Flora Kalogeropoulou, Zacharoula Zampeti, Anna Karantoni*

Laboratory of Organic Chemistry, School of Chemical Engineering, National Technical University of Athens, GREECE

Abstract

Biocompatible nanosystems and materials are currently gaining ground as potential tools for biomedical applications. Enhancement of the green character of nanosystems is a very important issue that can be addressed by taking several actions. The use of biodegradable and non-toxic natural polymers, such as chitosan, alginate, cellulose, etc. as well as oligomers such as cyclodextrin, as matrices for the encapsulation of bioactive compounds and/or natural products confers a greener character to the nanosystems, thus making a step towards more sustainable and safer materials. In addition, the use of toxic solvents and additives during the preparation of the nanosystems can be confined, and greener alternatives should be considered.

Essential oils (EOs), the multi-component mixtures obtained from aromatic plants comprising mainly low-molecular-weight metabolites such as terpenoids, phenolic compounds, and aliphatic components, possess a diverse array of biological activities, including antibacterial, antioxidant, antifungal, and antiviral properties. EOs are widely used in food preparations, mainly as natural preservatives and antimicrobials.

The combination of natural polymers and oligomers with EOs can offer a greener and more sustainable pathway towards biocompatible nanosystems and materials for a wide array of applications. In the present work, we will elaborate on the research conducted on the encapsulation of essential oils, extracted from aromatic plants and fruit, in various matrices and the potential of the produced nanosystems to act as antimicrobials and as pesticides.

Acknowledgement

This work has been produced with the financial assistance of the European Union under the Interreg NEXT MED Programme within the framework of Project No. A_T_1.1_0167-EONANOBIOPS ‘Essential Oil-derived Next Generation Nano-Biopesticides for Sustainable Eco-Friendly Agriculture’.

ORAL TALK

Real-World Performance of AI for Diabetic Retinopathy Screening

Abhinav Premkumar[1], Janvi Garg[2], Rithvik Inamapudi[1], Pranjal Sabuwala[1], Raga Battu[1]*

[1]Advocates in Technology Leadership and Science (ATLAS), United States

[2]Columbia University Mailman School of Public Health, United States

Abstract

Autonomous and semi-autonomous artificial intelligence (AI) systems for diabetic retinopathy (DR) screening are increasingly being integrated into primary care and teleophthalmology workflows. However, comparative evidence regarding real-world diagnostic performance, imageability, and implementation outcomes remains fragmented. Using the web-based review platform Rayyan, we synthesised findings from 14 studies evaluating AI-assisted DR screening systems, including EyeArt, IDx-DR/LumineticsCore, SELENA, and iHealthScreen.

Across evaluated systems, sensitivity for referable DR ranged from 86–100%, with large real-world deployments commonly reporting sensitivities above 90% and specificity in the mid-80s to low-90s range. Negative predictive values consistently approached 95–100%. Ungradable image rates varied substantially across workflows, though dilate-if-needed protocols significantly improved imageability and reduced ungradable examinations. AI-supported screening workflows in primary care settings were also associated with markedly improved ophthalmology follow-up adherence after abnormal screening results. Despite strong diagnostic performance, national utilisation of AI imaging billing code CPT 92229 remained extremely limited between 2021 and 2023.

Current DR screening AI systems demonstrate high-sensitivity detection of referable disease and meaningful implementation potential in real-world clinical environments. Broader population-level impact is presently constrained more by adoption and reimbursement barriers than by diagnostic limitations.

ORAL TALK

Enhancing cardiovascular risk prediction with biomarkers, genetics, socioeconomic status, and machine learning

Arjun Paunikar1, Nandita Sriram1, Venkat Narra1, Srikrithi Appikatla1, Janvi Garg2*

1ATLAS Research Program, USA; 2Baylor University and Columbia University, USA

Abstract

Cardiovascular risk prediction models increasingly incorporate biomarkers, genetic tools, and machine learning, yet it remains unclear which additions meaningfully improve performance beyond standard clinical factors and how often psychosocial and socioeconomic variables are considered.

We systematically reviewed 40 primary studies that developed or validated multivariable prediction models for cardiovascular disease, coronary heart disease, stroke, heart failure, major bleeding, or mortality in adult populations from community cohorts and high-risk clinical settings. Using a structured extraction framework, we collected information on populations, outcomes, modelling methods, and performance metrics for standard clinical models compared with enhanced models including socioeconomic status, inflammatory or cardiac biomarkers, polygenic risk scores, or machine-learning techniques. Where at least two comparable contrasts were available, we synthesised changes in C statistics and continuous net reclassification improvement using random-effects meta-analytic methods.

Classical predictors, including age, sex, blood pressure, smoking, diabetes, lipids, and prior cardiovascular disease, remained the strongest determinants of risk across nearly all studies. None of the reviewed studies incorporated psychosocial measures such as depression or perceived stress, and only a minority modelled socioeconomic status, despite evidence that deprivation measures improved calibration and corrected systematic risk misclassification. Adding high-sensitivity C-reactive protein produced only modest gains in discrimination, whereas natriuretic peptides and high-sensitivity troponin generated larger improvements in heart failure and perioperative cohorts. Polygenic risk scores slightly improved prediction but generally produced small increases in C statistics. Machine-learning models typically matched or only marginally exceeded traditional regression approaches, with inconsistent reporting of calibration and external validation.

Contemporary cardiovascular prediction models remain heavily dependent on classical clinical variables while underutilising socioeconomic and psychosocial determinants of health. The most clinically meaningful gains arise from selected high-yield biomarkers and explicit modelling of socioeconomic status, whereas broad machine-learning approaches and polygenic scores usually provide only modest improvements in discrimination.

ORAL TALK

AI-Assisted Diagnosis, Access, and Equity in Squamous Cell Carcinoma

Siddarth Mothukuri, Swaroop Kadiyam, Ritvika Venkatraman, Saisreeda Vutkuri, Janvi Garg*

ATLAS Research Program, Dallas, TX, USA

Abstract

Background: Artificial intelligence (AI)-assisted diagnostic systems are increasingly being deployed to improve skin cancer detection and expand specialist-level diagnostic capacity. However, their impact on healthcare disparities among low-income patients with squamous cell carcinoma (SCC) remains unclear.

Objective: To evaluate how AI-assisted diagnostic systems influence disparities in treatment continuity, specialist access, and downstream health outcomes among low-income U.S. adults newly diagnosed with SCC.

Methods: A structured evidence synthesis was conducted across 16 studies published between 2006 and 2025. Data were extracted using a standardised 47-field framework encompassing AI interventions, diagnostic performance, access measures, clinical outcomes, financial toxicity, quality-of-life metrics, equity indicators, and risk of bias. Studies were assessed using ROBINS-I, QUADAS-2, PROBAST, and Newcastle-Ottawa instruments where applicable. Sample-size-weighted pooled estimates were calculated when comparable outcomes were available.

Results: AI diagnostic performance was strong, with reported AUCs ranging from 0.630 to 0.968. In primary care settings, DermaSensor-assisted physicians demonstrated improved diagnostic sensitivity (+10.6 percentage points) and referral sensitivity (+9.4 percentage points) compared with unaided physicians. Teledermatology pathways increased access among Medicaid, Hispanic, and Black patients while reducing no-show rates. However, substantial baseline disparities persisted, including later-stage presentation, longer treatment delays, and worse survival among low-income and minority populations. Evidence regarding financial toxicity and post-treatment well-being was extremely limited, and no study directly evaluated quality-of-life outcomes in AI-exposed SCC cohorts. Training datasets frequently lacked adequate representation of darker skin tones and underserved populations.

Conclusions: Current evidence demonstrates strong diagnostic performance for AI-assisted SCC detection but limited evidence that these technologies reduce healthcare disparities. While primary-care deployment of AI tools may improve access, inadequate dataset diversity, reimbursement barriers, and the absence of patient-centred outcomes research raise concerns that AI implementation could unintentionally widen existing disparities. Future studies should

prioritise equity-focused validation and prospective assessment of financial and quality-of-life outcomes.

ORAL TALK

Tracking Inflammation Markers Prevents Early Death and Complications in Lung Cancer Immunotherapy

Twesha Singh, Sriram Siva, Shivam Loyalka, Tanvi Chakka, Janvi Garg*

ATLAS Research Program, Dallas, TX, USA

Abstract

Background: Systemic inflammation and nutritional status strongly influence prognosis and treatment response in non-small cell lung cancer (NSCLC), particularly among patients receiving immune checkpoint inhibitors (ICIs). Multiple recent studies have evaluated inflammatory cytokines, C-reactive protein (CRP), albumin-based indices, neutrophil-to-lymphocyte ratio (NLR), prognostic nutritional index (PNI), and related clinical outcomes.

Methods: A structured literature synthesis was conducted examining cohorts of advanced and resected NSCLC patients. Data regarding inflammatory biomarkers, composite prognostic scores, dynamic on-treatment changes, early mortality, immune-related adverse events, and metabolic consequences of inflammation were extracted and qualitatively synthesized. Reported hazard ratios, odds ratios, survival outcomes, and predictive performance metrics were evaluated.

Results: Advanced NSCLC patients demonstrated significantly elevated inflammatory cytokines, including IL-6, IL-8, IL-10, and TNF-RI, compared with controls. Elevated IL-6 was associated with substantially shorter overall survival and evidence of T-cell exhaustion. CRP-albumin–based scores, including the Glasgow Prognostic Score (GPS), modified GPS, CRP-to-albumin ratio (CAR), and PNI, consistently predicted poorer survival and increased recurrence risk, with hazard ratios commonly ranging from 2 to 4. Dynamic improvements in NLR and PNI following initiation of immunotherapy, summarized through the IMMUNO-SCORE, were associated with markedly improved treatment response and six- to sevenfold longer median survival, achieving an area under the curve of approximately 0.79 for predicting bone metastasis response. Early mortality within 60 days of ICI initiation occurred in approximately 13% of patients and was strongly associated with liver metastases and poor performance status. Acute kidney injury occurred in nearly one-quarter of ICI-treated patients and was independently associated with inflammatory and renal biomarkers.\

Conclusions: Inflammatory biomarkers and composite scores incorporating CRP, albumin, NLR, and PNI demonstrate strong and clinically meaningful associations with treatment response, survival, recurrence, early mortality, immune-related complications, and metabolic dysfunction in NSCLC. Dynamic monitoring of these markers may provide practical tools for risk stratification, treatment individualisation, and supportive care planning in patients undergoing immunotherapy.

DAY – 3, ROOM - B

INVITED TALK

Recycling NdFeB Magnets

Pierre Bernstein1, Abdelilah Chetouani2, Jean-Marie Le Breton2, Yiteng Xing1, Jérôme Lecourt1, Jacques Noudem2*

1 Normandie University, ENSICAEN, UNICAEN, CNRS, CRISMAT, Caen, France ;

2 Univ Rouen Normandie, INSA Rouen Normandie, CNRS, Normandie Univ, GPM UMR 6634

Abstract

NdFeB magnets are essential for many applications, such as electric cars, wind turbines and computer hard discs. The quantity of the Nd-Fe-B material used in applications ranges from 1 g in small electronics to 1 kg in electric vehicles and up to several tons in wind turbines. Their exceptional magnetic properties arise from the spin–orbit coupling between the 3d atomic orbitals of transition metals and the 4f orbitals of rare-earth elements, leading to strong orbital moments and high magnetisation. Their production, however, is strongly dependent on the availability of Nd, which, like the other Rare-Earths, is dependent on commercial and political contingencies. As a consequence, many countries and international organisations, such as the European Union, have set as a priority the recycling of disaffected artefacts containing Rare-Earths. While some efforts are dedicated to the direct recovery of the rare-earth elements by chemical processes, we have investigated the possibility of sintering new magnets from disaffected ones. For this purpose, the magnets were first turned into a powder by different techniques. The obtained powders were subsequently sintered by Spark Plasma Sintering (SPS), which is a non-conventional technique combining the application of a high mechanical pressure with a strong pulsed or direct current to the powder. SPS presents the advantages of short processing times, in the range of a few tens of minutes instead of hours for classical sintering, while resulting in high-density consolidated bulks. The hysteresis cycles of the obtained samples were recorded. The sought-after characteristics of the recycled magnets are a large coercive field and remanent magnetisation as well as a high energy product, also called grade, which is a figure of merit accounting, in particular, for the rectangularity of the cycle. In this contribution, we'll present the results obtained with the different processes investigated for producing powder, as well as the role of the mechanical pressure, atmosphere, temperature and duration of the sintering process. The coercive field of the recycled magnets has turned out to be very sensitive to oxidation, which reduces it strongly if it occurs at any stage of the recycling process. This problem could be alleviated by a post-annealing stage, but at the price of a deteriorated cycle

rectangularity. We'll show that the characteristics of the best recycled magnets meet those required for some applications, and we'll indicate possible solutions to improve them.

INVITED TALK

Computational Screening of High-Entropy Alloys for Hydrogen Storage Using HEAPS and MH Pro Programs

Afaf Ghais Abadi Ahmed, Asma Alhattali, Nouf Al-Rajhi, Wejdan Al-Isaee, Waad Al-Saadi, Eman Al Mamari*

University of Technology and Applied Sciences, Oman Afaf Ghais Abadi Ahmed

Abstract

Hydrogen storage is a critical component of the hydrogen energy chain for sustainable energy transfer and utilisation. Solid metals, particularly high-entropy alloys (HEAs), have emerged as promising materials for hydrogen storage due to their unique structure and thermodynamic properties. These properties arise from the mixing of four or more elements in a solid-solution alloy, which creates diffusion pathways for hydrogen absorption and desorption.

This work introduces computational models such as the High-Entropy Alloys Predicting Software (HEAPS) and the machine-learning-powered Metal Hydrides Pressure–Composition–Temperature Isotherm Predictor (MH-PCTpro) to accelerate the screening of HEAs suitable for hydrogen storage at low temperatures and atmospheric pressure. HEAPS was employed to generate initial structures and compositions for 200 candidate alloys, applying essential descriptors such as Valence Electron Concentration (VEC), atomic size mismatch, electronegativity difference, and mixing entropy to predict the solid solution structures favourable for hydrogen storage.

After structure generation, MH-PCTpro was used to validate hydride phase behaviour and assess hydrogen storage performance, including hydrogen uptake capacity and phase transition tendencies. Results indicate that BCC-type HEAs validated through MH-PCTpro exhibit superior hydrogen storage capacity (>2.0 wt%) and structural stability compared to FCC systems, which offer better reversibility.

By combining HEAPS for systematic structure generation with MH-PCTpro for detailed hydride-phase evaluation, this work bridges computational design with experimental feasibility, providing a scalable strategy for developing advanced hydrogen storage materials and supporting global efforts toward clean and sustainable energy technologies.

INVITED TALK

Evaluation of Mechanical Properties of Kenaf Core Fiber /UREA Formaldehyde Composites

*Saad A. Mutasher*1, Ekhlas A. Osman1, Tay Chen Chiang2*

1Department of Engineering and Technology, University of Technology and Applied Sciences

Suhar, Sultanate of Oman

2School of Engineering Computing and Sciences, Swinburne University of Technology (Sarawak Campus) 93350, Kuching, Sarawak, Malaysia

Abstract

This study focuses on utilizing kenaf core fiber with low-emission urea formaldehyde (UF) resin containing 51.6% solid content. Single-layer particleboard production was fabricated using kenaf core at two specified density levels: 500 kg/m³ and 600 kg/m³. Fiber weight fractions of (90%, 85%, 80%, 75%, 70%) were employed for both density types in the fabrication of kenaf UF composite boards. Various tests were conducted on each density type with the selected fiber weight fractions to assess the properties of the fabricated boards. The test results indicate that samples with higher density exhibit superior values for modulus of rupture, modulus of elasticity, tensile strength, Young's modulus, screw test, and internal bonding. Particleboards 500kg/m3 with 80 wt% and 600kg/m3at (70, 75, 80, 85) wt% had exceeded the M-1 and M-S specifications of American National Standard A208.1-2009 for wood particleboards. The M-1 and M-S classes of particleboard can be used as commercial products. Particleboard 500kg/m3 with 80wt% and all the 600kg/m3fulfilled the M-O standard. However, only the 600kg/m3 met the M-2 standard, which was for industrial purposes. Furthermore, the findings highlight the significant impact of density on board performance, as lower-density boards exhibit reduced mechanical strength compared to their higher-density counterparts.

ORAL TALK

Preliminary Correlation of LSCF Particle Size and Conformation Viability in Freeze-casting Processing [Sentence Case; Bold; Calibri 14]

[Note: Please use the font "Calibri 12", unless specified]

Natália Mata Oliveira2 , Amanda Assunção Rosa Silva1 , Mariana Lumi Ichihara Sado2 ,*

Carlos Martins Aiube1 , Rodrigo Nunes de Souza2 , Alysson Martins Almeida Silva2

1 Institute of Chemistry, Campus Darcy Ribeiro, University of Brasília – 70910-900. 2

Mechanical Engineering Department, Campus Darcy Ribeiro, University of Brasília – 70910-900

Abstract

Perovskites are a widely studied class of ceramic materials due to their structural and functional versatility and are applied in fuel cells, electrochemical devices, and gas permeation processes. Among them, mixed ionic and electronic ceramics, such as LSCF, have stood out for their essential properties for gas separation membranes. In this work, LSCF ceramic membranes were synthesised using the EDTA-citrate method, varying the calcination parameters to obtain different particle sizes. In addition, the membranes were conformed by the freeze-casting process, where parameters such as freezing temperature and mould geometry were adjusted to influence the final pore structure. The samples were characterised by X-ray diffraction (XRD), scanning electron microscopy (SEM), and micro-computed tomography (μCT). In addition, the Halder-Wagner, Scherrer, and Archimedes methods were applied to determine crystallite size, lattice tension, and porosity (open, closed, and total), respectively. The results indicated that the calcination time significantly influenced the crystallinity and particle size. XRD analysis revealed a rhombohedral perovskite structure, while increasing the thermal treatment time promoted changes in the crystallite size and lattice tension. SEM showed a homogeneous distribution of the elements and a reduction in the grain size as the parameters in the calcination process changed. Freeze-casting in geometries such as disks is being investigated and optimised to obtain membranes with anisotropic structures and controlled pore alignment, highlighting the importance of thermal control in optimising the structural properties of the membranes. Thus, the findings of this work provide relevant information for the optimisation of the production and forming process of perovskite-based ceramic membranes, aiming at greater mechanical and chemical stability for applications in gas separation.

Acknowledgements: This work was supported by Petronas, UnB e CAPES

INVITED TALK

3D Bioprinting of a Cardiac Patch Using Decellularised Bovine Pericardium, Silk Fibroin, and Gold Nanoparticles

Yüksel Çetin1, Ayşenur Atak2, Ayşen Güngör3, Ayça Bal Öztürk3,4,5*

1Life Sciences, Biotechnology Unit, TUBITAK MAM, Kocaeli, Türkiye; 2Molecular Biology and Genetics, Yildiz Technical University, Istanbul, Türkiye; 3Department of Stem Cell and Tissue Engineering, Institute of Health Sciences, Istinye University, Istanbul, Türkiye; 4Stem Cell and Tissue Engineering Application and Research Center (ISUKOK), Istinye University, Istanbul, Türkiye; 5Department of Analytical Chemistry, Faculty of Pharmacy, Istinye University, Istanbul, Türkiye

Abstract

Cardiovascular diseases (CVDs) remain the leading cause of mortality worldwide, accounting for approximately 17.5 million deaths annually, with projections exceeding 23.6 million by 2030. Current clinical solutions for cardiac repair, including synthetic and biological

implants, are limited by immunogenicity, calcification, inflammation, thromboembolic complications, insufficient electrical conductivity, and poor long-term functionality. The primary aim of this study is to develop a biocompatible, anti-immunogenic, biodurable, conductive, and biomimetic 3D cardiac patch that mimics the native cardiac microenvironment and promotes cardiac regeneration. A composite bioink was engineered using decellularised bovine pericardium as a natural extracellular matrix scaffold, silk fibroin to enhance mechanical strength and reduce calcification, and gold nanowires to confer electrical conductivity and mechanical reinforcement. The cardiac patch was fabricated using 3D bioprinting technology. Nanobiotechnological, biochemical, mechanical, and electrophysiological characterizations were performed. Biodegradability and biocompatibility were evaluated in accordance with ISO 10993 medical device standards. The developed cardiac patch provided a biomimetic 3D microenvironment that supported cardiac cell adhesion, proliferation, differentiation, and endothelization. The integration of gold nanowires was anticipated to improve electrical signal propagation and mechanical stability, thereby reducing risks of aneurysm, calcification, infection, and post-surgical bleeding. The results confirmed that the developed functionally advanced, living cardiac patch is a promising medical device to overcome current clinical limitations in cardiovascular implants.

ORAL TALK

Nanoarchitectonics of Fullerene-derived Carbon: Cavity Engineering in Fullerene Self-assembly for Ammonium-ion Storage

Sabina SHAHI1,2,, Katsuhiko Ariga1,3, Lok Kumar Shrestha1,2**

1Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba 305-0044, Japan, 2Department of Materials Science, Institute of Pure and Applied Sciences, University of Tsukuba; 1-1, Tennodai, 305-8573 Tsukuba, Ibaraki, Japan, 3Department of Advanced Materials Science, Graduate School of Frontier Sciences, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8561, Japan

Abstract

Ammonium-ion hybrid supercapacitors have recently emerged as efficient and sustainable electrochemical energy storage systems, primarily due to the smaller hydrated ionic radius of NH4+, rapid ion diffusion kinetics, and environmental safety. The current study focuses primarily on cathode materials, with limited attention to anode materials. Here, we discuss fullerene-based porous hollow carbon spheres as an anode material for storing ammonium ions and systematically compare their performance with that of solid spheres to reveal the structure-property relationship. Self-assembled fullerene-derived hollow carbon spheres are promising due to their unique morphology, tunable nanostructure, high conductivity, and excellent thermal and chemical stability. Electrochemical results demonstrate that the hollow carbon spheres exhibit superior energy storage performance, highlighting the importance of their hollow architecture in enhancing performance. Owing to their high specific surface area

(1800 m2 g-1) and hierarchical micro/mesoporous structures, hollow carbon spheres anode achieved an excellent gravimetric capacitance of 134 F g-1 at a current density of 0.5 F g-1, which demonstrates them as a promising anode material for ammonium-ion storage. Finally, we will also discuss our recent results on the design of novel composite materials by integrating pseudocapacitive metal oxides into higher-dimensional fullerene-derived porous carbon materials.

ORAL TALK

Biomass Nanoarchitectonics: Sustainable Porous Carbon Materials for Energy Storage Applications

Aabha Puri1,2,, Katsuhiko Ariga1,3, and Lok Kumar Shrestha1,2*

1Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba, Ibaraki, 305-0044, JAPAN

2Department of Materials Science, Institute of Pure and Applied Sciences, University of Tsukuba 1-1-1, Tennodai, Tsukuba, Ibaraki, 305-8573, JAPAN

3Department of Advanced Materials Science, Graduate School of Frontier Sciences, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8561, JAPAN

Abstract

The rapid growth of the global economy has intensified fossil fuel consumption, leading to resource depletion and environmental concerns, thereby accelerating the demand for renewable energy systems and efficient energy storage technologies. Supercapacitors are promising energy storage devices due to their high power density, rapid charge–discharge capability, long cycle life, and excellent rate performance; however, their relatively low energy density remains a critical limitation. To address this challenge, the rational design of sustainable, high-performance electrode materials through simple and scalable synthesis strategies is essential. Herein, we report the fabrication of high-surface-area, self-heteroatom-doped porous carbon derived from the sustainable biomass Achyranthus bidentata. The porous structure was tailored by optimising the carbonisation temperature, the type of activator, and the impregnation ratios. The optimised material (KOH-activated at 900 °C at a 1:1 ratio) exhibited an ultra-high surface area of 2251 $m^2\ g^{-1}$, partial graphitisation, and retained surface heteroatoms, which contribute to enhanced electrochemical activity. Electrochemical evaluation in a three-electrode configuration showed a specific capacitance of 265 F g^{-1} at 1 A g^{-1} in an aqueous electrolyte. Furthermore, a symmetric supercapacitor assembled with the optimised electrode delivered an energy density of 9.3 Wh kg^{-1} at a power density of 700 W kg^{-1}, along with excellent cycling stability. These findings present a facile, sustainable, and scalable strategy for converting biomass waste into high-performance porous carbon electrodes, highlighting their strong potential for next-generation energy storage applications.

ORAL TALK

The Psychology of Web Design: A Case Study about the Contemporary Challenges between Neuroscience and Technology.

Pedro Cauã Galdino Lima[1], Denise Silva do Amaral[2], Mairon Santana do Nascimento[3], Maria Clara da Silva Santiago 4, Maria de Deus Das Chagas Souza 5, Gustavo Carneiro de Lima Botelho6*

[1]Instituto Federal de Ciência e Tecnologia do Ceará, Brazil; [2]Instituto Federal de Ciência e Tecnologia do Ceará, Brazil; [3]Instituto Federal de Ciência e Tecnologia do Ceará, Brazil; 4 Instituto Federal de Ciência e Tecnologia do Ceará, Brazil; 5Instituto Federal de Ciência e Tecnologia do Ceará, Brazil; 6 Instituto Federal de Ciência e Tecnologia do Ceará, Brasil.

Abstract

With the increasing presence of digital platforms in the population's routine, interactive design has demonstrated a deeper impact on the behaviour of individuals. In this context, there's still a limited comprehension of the mechanisms used by big techs to stimulate compulsive and constant engagement. The objective of this study is to investigate the psychology applied to web design, focused on the analysis of behavioural design to induce decisions and emotions in users; the present research tries to understand how the design and interactive elements influence the routine and perception. The chosen methodology consists of a mixed approach, combining a bibliographic review and a quantitative field research. In the bibliographic revision, theoretical models like “Hooked” by Nier Eyal, the impact of the internet and social media on society's behaviour, and the regulation of digital platforms were analysed and studied. The field research was introduced with the application of a formulary to the students of the secondary school ‘EEEP Professora Elsa Maria Porto Costa Lima’, and the collected data were analysed through percentual calculus to identify patterns of use, erception, and the impact of technologies on the routine of the teenagers. The application of the research identified a pattern of intensive general usage of mobile devices, with all teenagers (100%) affirming usage with a frequency of five days or more per week, followed by an elevated daily usage time. The students' perceptions about the digital immersion were ambiguous; the predominant feelings with the high usage were "Indifferent" (52%) or "Positive" (48%), with none affirming negative feelings like stress or anguish.

Although 40% of the students affirmed they perceive that their routine is being disturbed by frequent contact with mobile devices, they do not affirmatively perceive negative impacts in the way they feel while using them. Hence, the analysed data corroborate with the efficacy of Comportamental Design, aligned to “Hooked Model”, in the creation and maintenance of intensive digital habits. Those implications reveal the inert state that the users are in, given the daily use of mobile devices and the unawareness or loss of perception of the negative impact on their emotions, suggesting a normalisation of those behaviours and a possible difficulty in associating the intensive usage with adverse consequences.

Therefore, it's important to bring up discussions about the regulation of social media to mitigate the potential compulsive effects and to grant a healthier digital space to all of the users.

ORAL TALK

Dy3+-Activated BaYAl3O7 under UV Excitation: A Promising Phosphor for Therapeutic Functional Composites

Aabha Pardhi1 , Nameeta Brahme1, D. P. Bisen1,Kiran Varma1, Garima Dewangan1

1S.o.S. in Physics and Astrophysics, Pt. Ravishankar Shukla University, Raipur.

Abstract

The development of functional and smart composites capable of delivering both structural integrity and active, human-centric functionalities has become increasingly important for next-generation materials. In this study, a Dy3+-activated BaYAl3O7 luminescent ceramic is engineered as a multifunctional phosphor for integration into advanced composite systems targeting therapeutic light delivery. The material was synthesised via a high-temperature solid-state reaction (1200 °C for 8 h), resulting in a composite crystalline framework comprising hexagonal BaAl2O4 and orthorhombic YAlO3 phases. Structural analysis using X-ray diffraction confirms high crystallinity, phase stability, and successful incorporation of Dy3+ions within the host lattice, with an average crystallite size of approximately 51.6 nm. Upon UV excitation at 358 nm—well aligned with commercially available UV-LED sources—the phosphor exhibits strong dual-emission bands in the blue (465 nm,4F9/2 →6H15/2) and yellow (580 nm, 4F9/2 → 6H13/2) regions, enabling efficient UV-to-visible energy conversion. These findings establish a viable strategy for embedding luminescent ceramic nanophases into functional composite architectures, facilitating controlled light-mediated biological interactions. The developed Dy3+-doped BaYAl3O7 system demonstrates significant potential for applications in biomedical devices, wearable phototherapy platforms, and human-centric multifunctional materials.

Keywords: Luminescent ceramics, Dy3+ phosphor, therapeutic light, Solid-state synthesis, Functional composites

---

PRISM

PROFESSIONAL CONFERENCE ORGANIZERS

Prism Scientific Services Pty Ltd., a premier conference organizer, envisions a sustainable future for the Science and Engineering. Our goal is to unite experts and stakeholders through conferences, fostering collaboration and advancing sustainable practices. Committed to curating conferences on materials science, renewable energy and eco-friendly technologies, we catalyze the industry's development. Emphasizing interdisciplinary collaboration, our events address complex challenges. Dedicated to sustainability, we minimize footprints and promote eco-friendly venues, inspiring environmental responsibility. As catalysts for positive change, guiding the energy industry toward an innovative, environmentally responsible future in conferences that prioritize sustainable development.

If you are interested in forming a partnership with us for the planning and organization of conferences and events worldwide, please don't hesitate to contact us via email at **writeus@scientificprism.com** or by phone at **+61 416000202.** Our services extend to facilitating conferences anywhere in the world, and we look forward to the opportunity to discuss your specific needs and requirements.

WE WISH TO SEE YOU AT MATERIALS EUROPE-2027

PRISM

akshatha@materialsconferenceeurope.com
Australia: +61 390163202
Prism Scientific Services Pty Ltd
302/480 Collins Street, Melbourne, VIC 3000, Australia
www.scientificprism.com

www.materialsconferenceeurope.com