



6th International Conference on Nanomaterials Science and Mechanical Engineering

University of Aveiro, Portugal

July 9-12, 2024

Book of Abstracts

**tema**

university of aveiro

centre for mechanical technology and automation

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6th International Conference on Nanomaterials Science and Mechanical Engineering
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6th International Conference on Nanomaterials Science and Mechanical Engineering

University of Aveiro, Portugal

July 9-12, 2024

(6th ICNMSME-2024)

looks for significant Modern Problems of Nanomaterials Science and Mechanical Engineering, to provide a platform to the global researchers and practitioners from both academia as well as industry to meet and share cutting-edge development in the fields, to give possibility for young scientists and students present results and find your place in the future world.

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ICNMSME2024 program

July 9, 2024 (Tuesday)

2nd Workshop on New Challenges of Bionanomaterials: Science, Technology, Application University of Aveiro, Portugal, 9 July, 2024	
9:00–9:10	WELCOME ADDRESS Dr. Gil Gonçalves Dr. Igor Bdikin
9:10–9:40	CHAIR: Dr. Gil Gonçalves and Dr. Igor Bdikin W3-O1. Addressing the ecotoxicity of micro(nano)plastics of polyhydroxybutyrate (biobased) and polymethylmethacrylate (petroleum-based) on <i>Danio rerio</i> physiology and behaviour Cátia Venâncio <i>Centre for Environmental and Marine Studies, Department of Biology, University of Aveiro, 3810-193 Aveiro, Portugal</i>
9:40 – 9:55	W3-O2. Protein-based nanomaterials as magnetic resonance imaging contrast agents Gabriela Guedes <i>Center for Cooperative Research in Biomaterials (CIC biomaGUNE), Basque Research and Technology Alliance, Parque Tecnológico de San Sebastian Paseo Miramón 194, 20014 Donostia-San Sebastian, Spain</i>
9:55 -10:10	W3-O3. Development of biobased polyesters derived from 2,5-furandicarboxylic acid and their sustainable nanostructures Lorenzo Ceparano <i>CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal</i>
10:10 – 10:25	W3-O4. A case study comparing the impacts of nanometric particles made of petroleum and biopolymers on freshwater organisms Miguel Oliveira <i>Centre for Environmental and Marine Studies, Department of Biology, University of Aveiro, 3810-193 Aveiro, Portugal</i>



10:25 – 10:45	Coffee break / Open discussions
Workshop on “ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES” (9 July 2024)	
10:45–10:55	WELCOME ADDRESS Dr. Indrani Coondoo Prof. Georgina Miranda
10:55–11:30	CHAIR: Dr. Indrani Coondoo <i>Keynote talk</i> Functionalized nanofibers by electrospinning For Energy applications Prof. Bernardo Almeida University of Minho, Portugal
11:30–12:15	<i>Plenary Lecture</i> 3D Printed Porous Ceria Ceramics for Solar Thermochemical Production of Sustainable Fuels Prof. Robert Pullar Università Ca' Foscari Venezia, Italy
12:15–14:00	Lunch
14:00–14:30	<i>Keynote talk</i> One-dimensional charge transporting columnar mesogens for optoelectronic applications Dr. Dharmendra Pratap Singh Université du Littoral Côte d’Opale (ULCO), France



2nd International Workshop on “Modern Trends in Energy Research”, University of Aveiro, Portugal, July 9, 2024 (IWMTER-2024) Affiliation of workshop speakers: Centre for Mechanical Technology and Automation – TEMA, Department of Mechanical Engineering, University of Aveiro, Portugal Session Chairs: Dr. Duncan Paul Fagg / Dr. Laura Holz	
14:30–15:00	WELCOME ADDRESS and workshop introduction D. Pukazhselvan
	<u>Planary Lecture:</u> Highlights to the advanced anode active materials for rechargeable batteries D. Pukazhselvan
15.00–15.20	<u>Invited Talk-1:</u> Electrospun $[\text{Ca}_2\text{CoO}_{3-\delta}]_{0.62}[\text{CoO}_2]$ nanofibres: Improving the oxygen reaction kinetics in solid oxide fuel cell cathodes Allan J. M. Araújo
15.20–15.35	<u>Invited Talk-2:</u> Synthesis of novel electrolytes for proton ceramic membrane Reactors Alfredo S. B. Luemba
15.35–15.50	<u>Invited Talk-3:</u> Low-Cost $\text{Ca}_2\text{Fe}_2\text{O}_5$ Catalysts Synthesized by Reactive Firing of Calcite and Siderite for Application in Alternative Energy Technologies Isabel Antunes
15.50–16.10	Coffee break / Open discussions
16:10–16:30	<u>Planary Lecture:</u> Thermogravimetry: how to build a kinetic model. A case study of the oxidation of niobium nitride Vanessa Graça
16:30–16:45	<u>Invited Talk-4:</u> Life cycle assessment of energy-dense fuels from electrochemical biogas conversion J.K. Ravindran
16:45–17:00	<u>Invited Talk-5:</u> Harnessing Energy from Salinity Gradients through Reversible Electrodialysis Eduardo Durana
17.00–17.20	<u>Invited Talk-6 / Keynote address and closing remarks</u> Proton conductivity in doped barium cerate under nominally dry conditions Francisco JA Loureiro



5th Workshop on Characterization and Analysis of Nanomaterials
University of Aveiro, Portugal, July 9, 2024

17:20-17:30	WELCOME ADDRESS Dr. Igor Bdikin, Dr. Gil Gonçalves
17:30-17:55	CHAIR: Dr. Igor Bdikin and Dr. Laura Holz <i>Keynote talk</i> W1-I1. X-ray diffraction (XRD) Dr. Laura Holz University of Aveiro, Aveiro, 3810-193, Portugal
17:55-18:30	<i>Plenary Lecture</i> X-ray Microtomography for materials characterization Prof. Dr. Isabel Duarte University of Aveiro, Aveiro, 3810-193, Portugal
18:30-19:00	W1-O1. Atomic force microscopy (AFM) Dr. Igor Bdikin University of Aveiro, Aveiro, 3810-193, Portugal
19:00-19:15	Close/discussions



July 10, 2024 (Wednesday)

6th International Conference on Nanomaterials Science and Mechanical Engineering (6th ICNMSME-2024)	
9:00-9:10	WELCOME ADDRESS: Prof. Dr. Robertt Angelo Fontes Valente (UA, Portugal), Prof. Dr. Vítor António Ferreira da Costa (UA, Portugal), Prof. Dr. António Manuel de Bastos Pereira (UA, Portugal), Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques (UA, Portugal), Dr. Duncan Paul Fagg (UA, Portugal), Dr. Igor Bdikin (UA, Portugal), Dr. Gonzalo Guillermo Otero Irurueta (UA, Portugal), Dr. Gil Alberto Batista Gonçalves (UA, Portugal)
9:10-9:30	Session: New Materials and Advanced Materials CHAIRS: Dr. Natália Barroca , Dr. André Girão Keynote talk Dr. Oleksandr Tkach (I24) Properties of Li- and Mn-doped Potassium Tantalate Polar Dielectrics <i>Department of Materials and Ceramic Engineering, CICECO – Aveiro Institute of Materials, University of Aveiro, Aveiro 3810-193, Portugal</i>
9:30-9:45	Session: Composites Prof. Dr. Martina Kocijan (O3) Photocatalytic degradation of methylene blue using carbon-based materials <i>Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Ivana Lučića 5, 10000 Zagreb, Croatia</i>
9:45-10:00	Coffee break
10:00-10:40	Session: Sensors and Actuators Plenary Lecture Prof. Dr. Senentxu Lanceros-Méndez Sustainable Approaches for Printable Sensors and Actuators <i>BCMaterials, Basque Center for Materials, Applications and Nanostructures, UPV/EHU Science Park, 48940 Leioa, Spain</i> <i>IKERBASQUE, Basque Foundation for Science, 48009 Bilbao, Spain</i>



10:40-11:00	Session: Hydrogen and Fuel Cell Science Keynote talk Dr. Laura Holz (I18) Synthesis and Characterization of CO₂-Stable Yttrium-Doped BaZr_{0.8-x}Sn_xY_{0.2}O_{3-δ} Proton-Conducting Electrolytes <i>TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal</i>
11:00-11:15	Session: Hydrogen and Fuel Cell Science Aleksandr Bamburov (O30) Enhancing efficiency of solid oxide electrolysis cells through carbon-assisted approach: Materials characterization and performance analysis <i>CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal</i>
11:15-11:30	Session: Hydrogen and Fuel Cell Science Rui Pinto (O4) Perovskite Anodes for Biogas-Powered SOFCs: CaVO₃, SrVO₃, SrMoO₃ <i>CICECO – Aveiro Institute of Materials, University of Aveiro, Aveiro, Portugal</i>
11:30-11:45	Session: Ceramics Diogo João Breda Lopes (O31) Laser Floating Zone as a tool for high temperature SrTiO₃ and TiO₂-based oxide thermoelectrics <i>CICECO - Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal</i>
11:45-12:00	Session: Ceramics Parisa Amirkhizi (O32) Enhancing Electrical Properties of Barium Titanate-Based Ceramic Thermoelectrics: Comparing Solid State Technique and Spark Plasma Sintering <i>Department of Materials and Ceramic Engineering, CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193, Aveiro, Portugal</i>
12:00-13:30	Lunch
13:30-14:00	Session: Hydrogen Storage CHAIRS: Prof. Dr. Vitor Neto, Dr. Oleksandr Tkach, Dr. Pavel Zelenovskii Keynote talk Dr. D. Pukazhselvan (I20) Reaching the reversible hydrogen storage target by regenerating the irreversible high capacity hydride LiBH₄ <i>Department of Mechanical Engineering, TEMAs - Centre for Mechanical Technology and Automation, University of Aveiro, Aveiro 3810-193, Portugal</i>



14:00-14:30	Session: Materials Science – Sensors Materials Plenary Lecture Prof. Dr. Ajeet Kaushik Emerging sensing Approach for health and Environmental management <i>Florida State University, USA</i>
14:30-14:50	Session: Thin films Keynote talk Prof. Dr. Neeraj Panwar (I7) Enhancement in ultraviolet photodetection of DyCrO₃/n-Si heterojunction devices with manganese substitution <i>Department of Physics, Central University of Rajasthan Bandarsindri, Ajmer-305817 Rajasthan, India</i>
14:50-15:10	Session: Hydrogen and Fuel Cell Science Keynote talk Prof. Dr. Francisco Loureiro (I9) Mixed ionic and electronic conductors for Solid Oxide Cells <i>TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal</i>
15:10-15:30	Session: New Materials and Advanced Materials Keynote talk Dr. Natália Barroca (I17) Strategies to interface an adipose-derived decellularized extracellular matrix with graphene-based materials for neural tissue engineering <i>Centre for Mechanical Technology Automation (TEMA), Department of Mechanical Engineering, University of Aveiro, Aveiro, Portugal</i>
15:30-15:45	Coffee break
15:45-16:00	Session: Biomaterials Dr. Joanna Fronczyk (O7) Enhancing MICP Self-Healing Concrete by Optimizing Carbonate Precipitation <i>Warsaw University of Life Sciences – SGGW, 166 Nowoursynowska Str., 02-787 Warsaw, Poland</i>
16:00-16:15	Session: Building Materials Dr. Caio C. dos Santos (O6) Rheological Properties of Cement Pastes Mixtures with Mixed Oxide Additives <i>São Paulo State University (UNESP) Araraquara, São Paulo, Brazil</i>
16:15-16:35	Session: Surface Engineering/Coatings Keynote talk Dr. Ana Violeta Girão (I25) Combining Electrochemical Deposition and PVD Coatings Towards Chromium (VI) Replacement <i>CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal</i>



16:35-16:50	Session: Thermal Engineering Theory and Applications Dr. AMIRAT Hamza (O34) The Influence of T-Shape Flow Deflector Placement on Convection Heat Transfer over an Array Heated Blocks <i>University of Yahia Fares, Laboratory of Mechanics, Physics and Mathematical Modeling (LMP2M) Medea, Algeria</i>
16:50-17:00	Session: New Materials and Advanced Materials Composites HAMMOUDI Hadda Aya (O8) Composite materials synthesis for dye adsorption: Optimization by Box-Behnken experimental design and implications for water treatment <i>Laboratory of Materials Technology, University of Science and Technology Houari Boumediene, B.P. 32, El-Alia, Bab-Ezzouar, Algiers, Algeria</i>
17:15-17:30	Session: Nanotechnology Khadija EL KALAAOUI (O14) Hybrid Polyvinyl Alcohol-Silica Antibacterial Nanofiber Fabricated by Combined Sol-Gel and Electrospinning Techniques <i>Laboratory of Engineering and Materials (LIMAT), Faculty of Sciences Ben M'Sik, Hassan II University of Casablanca, Casablanca, Morocco</i>
17:30-17:45	Session: Manufacturing Processes and Mechanical Engineering Luís Nascimento (O18) Towards Piezoelectric Oriented Fibrous Platforms for CTE: Establishing Principles for EHD Jet Printing <i>Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193, Aveiro, Portugal</i>
17:45-18:00	Session: Hydrogen and Fuel Cell Science Fardous Ajeeb (O33) Biogas conversion system for green liquid fuel production <i>TEMA, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal</i>



July 11, 2024 (Thursday)

6th International Conference on Nanomaterials Science and Mechanical Engineering (6th ICNMSME-2024)	
8:45-9:05	Session: Biomaterials CHAIRS: Dr. Andrei Kovalevsky and Dr. Gil Gonçalves Keynote talk Dr. Gil Gonçalves (I28) The bright future of Carbon Dots for biomedical and environmental applications <i>Department of Mechanical Engineering, University of Aveiro, Portugal</i>
9:05-9:25	Session: Sensor Materials Prof. Dr. Andrzej Kudelski (O1) DNA identification using surface enhanced Raman scattering (SERS): different types of SERS DNA sensors <i>Faculty of Chemistry, University of Warsaw, 02-093 Warszawa, Poland</i>
9:25-9:45	Session: Optical Materials Keynote talk Dr. Suresh Kumar Jakka (I6) Photoluminescent Active Ion-Doped Glasses for Advanced Gas Sensing Applications <i>I3N-Department of Physics, University of Aveiro, Aveiro, Portugal</i>
9:45-10:00	Session: Protective Coatings and Corrosion of Materials Amira Gharbi (O2) The beneficial effects of CeO₂ NPs integration on the microstructure and corrosion behavior of electrodeposited nickel coatings <i>Process Engineering Department, Physics of Matter and Radiation Laboratory LPMR, Mohamed Chérif Messaadia university, Souk Ahras 41000- Algeria</i>
10:00-10:15	Coffee break
10:15-10:30	Session: New Materials and Advanced Materials Amaia Zarandona Rodríguez (O29) Doping vs Functionalization: advanced modification strategies for enhanced sonophotocatalytic degradation of contaminants of emerging concern from water <i>BCMaterials, Basque Center for Materials, Applications and Nanostructures, UPV/EHU Science Park, 48940 Leioa, Spain</i>



10:30-10:50	Session: New Energy Materials Keynote talk Dr. Venkata Eskilla (I22) Organized functional nanomaterials for energy applications <i>I3N, Department of Physics, University of Aveiro, 3810-193, Aveiro, Portugal</i>
10:50-11:20	Session: Nanotechnology Keynote talk Prof. Dr. Ricardo J. B. Pinto (I27) Unveiling the impact of the size and morphology of levodopa-functionalized gold nanourchins in their in vitro cytotoxicity <i>CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal</i>
11:20-11:40	Session: New Energy Materials Keynote talk Prof. Dr. Sajid Hussain Siyal (I16) Energy Storage: Challenges of 21st Centuries and modification of Solid State electrolytes for next generation batteries <i>Dawood University of Engineering and Technology, M.A Jinnah Road Karachi, 74800 Sindh Pakistan</i>
11:40-12:00	Session: Materials Science - Engineering & Technology Keynote talk Dr. Caroline Maria Bezerra de Araujo (I21) Composite hydrogels based on graphene oxide and biopolymer as adsorbents: applications in separation processes <i>Centre of Chemistry, University of Minho Campus de Gualtar, 4710-057 Braga, Portugal</i>
12:00-13:30	Lunch
13:30-14:00	Session: Ceramics CHAIRS: Dr. Pavani Krishnapuram and Dr. D. Pukazhselvan Plenary Lecture Prof. Dr. Gunnar Suchaneck The origin of the low-temperature resistivity upturn in strontium ferromolybdate ceramics <i>Institute of Solid-State Electronics, TU Dresden, 01062 Dresden, Germany</i>
14:00-14:30	Session: CO₂ Utilization Plenary Lecture Prof. Dr. Salam J.J. Titinchi Supported catalysts for CO₂ cycloaddition reactions <i>Department of Chemistry, University of the Western Cape, Cape Town, South Africa</i>



14:30-15:00	Session: Biomaterials Keynote talk Prof. Dr. Serbürent Türk (I1) Development of Biopolymer-Based Hydrogels with Varying Porosity Ratio <i>Sakarya University, Biomedical, Magnetic and Semiconductor Materials Application and Research Center (BIMAS-RC), 54187 Sakarya, Turkey</i>
15:00-15:20	Session: Composites Keynote talk Prof. Dr. S. Shanmuga Sundari (I10) Effect of ion implantation in alkali borate glasses <i>Department of Physics, Seethalakshmi Ramaswami College, Trichy, 620002, India</i>
15:20-15:40	Session: Low Dimension Structures Keynote talk Prof. Dr. Alaa Almansoori (I12) Low-Voltage Scanning Electron Microscopy as a Crucial Tool for Optimizing the Properties of Polymer-Nanoclay Composites <i>Basrah Technical Institute, Southern Technical University, Basrah, Iraq</i>
15:40-16:00	Session: Ceramics Keynote talk Dr. Andrei Kovalevsky (I3) Sustainable thermoelectrics: the potential of strontium titanate <i>CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Portugal</i>
16:00-16:15	Coffee break
16:15-18:30	Poster Sessions (P1-P30)
20:00-21:30	Banquet



July 12, 2024 (Friday)

6th International Conference on Nanomaterials Science and Mechanical Engineering (6th ICNMSME-2024)	
9:00-9:20	Session: Micro / Nano Materials CHAIRS: Prof. Dr. Ricardo Pinto and Dr. Suresh Kumar Jakka Keynote talk Prof. Dr. Isabel Duarte (I5) Cellular Metals in Engineering Applications <i>Department of Mechanical Engineering, University of Aveiro, Portugal</i>
9:20-9:40	Session: New Materials and Advanced Materials Keynote talk Prof. Dr. Natalia Tintaru (I14) Electrospark alloying and Electrochemical Methods as Effective Technologies for Obtaining Advanced Materials <i>Laboratory of Electrophysical and Electrochemical Treatment of Materials Boris Lazarenko, Institute of Applied Physics, Moldova State University, MD-2028 Chisinau, Moldova</i>
9:40-10:00	Session: New Materials and Advanced Materials CHAIRS: Prof. Dr. Ricardo Pinto, Dr. Suresh Kumar Jakka Keynote talk Prof. Dr. Henrikas Cesiulis (I26) Metallic foams as a substrate in the electrochemical technologies <i>Vilnius University, Faculty of Chemistry and Geosciences, Naugarduko str. 24, Vilnius, Lithuania</i>
10:00-10:20	Coffee break
10:20-10:40	Session: Modeling/nanocomposite Keynote talk Prof. Dr. Jamal Davoodi (I19) Molecular dynamics simulation of graphene woven fabric/polyethylene nanocomposite <i>Faculty of science, University of zanzan, Zanzan, Iran</i>



10:40-11:00	Session: Optical Materials Dr. Sultan Ben Jaber (O28) Surface enhanced infrared absorption for detection of ultra-trace of 3,4- methylene dioxy-methamphetamine (MDMA) <i>Department of Criminal Justice & Forensic Science, King Fahad Security College, Riyadh 13232, Saudi Arabia</i>
11:15-11:30	Session: Optical Materials Keynote talk Dr. Pavani Krishnapuram (I8) Non-concentration quenching phenomena in red-emitting Eu³⁺ doped layered bismuth tungstate Aurivillius family compound <i>I3N-Department of Physics, University of Aveiro, Aveiro, Portugal</i>
11:30-11:45	Session: Micro / Nano Materials Bilal FETTAH (O9) Investigation of Damping in Porous Metal Foams <i>Laboratory of Rheology and Mechanics, Hassiba Benbouali University of Chlef, Algeria</i>
11:45-12:00	Session: Biomaterials Yağmur Camcı (O27) Development of Lyophilized Hydrogel/Nanofiber Composite Scaffold for Soft Tissue Engineering <i>Sakarya University, Biomedical Engineering, Institute of Natural Sciences, Esentepe Campus, 54187, Sakarya, Turkey</i>
12:00-13:30	Lunch
13:30-14:00	Session: Composites CHAIRS: Dr. Martina Kocijan and Dr. Venkata Esquilla Keynote talk Prof. Dr. Vikram Uttam Pandit (I2) Synthesis, Characterization and Photocatalytic applications of New Composite system <i>Haribhai V. Desai Arts, Science & Commerce College, Pune-411002, India</i>
14:00-14:30	Session: Waste-to-Energy Keynote talk Prof. Dr. Musaab ZAROG (I11) Shape Optimization for Broadband Vibration-based Piezoelectric Energy Harvesters <i>Department of Mechanical and Industrial Engineering, College of Engineering, Sultan Qaboos University, P.O. Box 33, Al-Khoudh, Muscat, 123, Sultanate of Oman</i>
14:30-14:45	Session: New Energy Materials Nahitcan Yilmaz (O10) The Sulfuric Acid Etching Effect of Fly Ash/SiO₂ as Anode for Li-ion Batteries <i>Department of Energy Resources and Management, Canakkale, Turkey</i>



14:45-15:00	Session: Design and Optimization of a New Type of Mechanical Heart Valve Rabia Güzide AL (O11) Optimizing Mechanical Heart Valve Efficiency: A Systematic Approach <i>Biomedical Engineering, Institute of Natural Sciences, Sakarya University, Esentepe Campus, 54187 Sakarya, Turkey</i>
15:00-15:15	Session: Stimuli Responsive Biomaterials Mahsa Heidarnejad (O12) Synthesis of chitosan-PVA hydrogel as a drug delivery system and in vitro loading and release studies of resveratrol <i>Sakarya University, Institute of Natural Sciences, Department of Chemistry, 54187, Sakarya, Turkiye</i>
15:15-15:35	Session: Low Dimension Structures Justyna Niewiadomska (O5) Structural variety of metals as a cause of the variety of oxidation states and coordination number: structural analysis of selected ruthenium complexes <i>tab edizioni, Viale Manzoni 24c, 00185, Rome, Italy</i>
15:35-16:00	Coffee break
16:00-16:20	Session: Thin Films Keynote talk Prof. Dr. Aleksandr Bagmut (I15) Crystallization modes in amorphous films of V_2VI_3 semiconductors according to TEM with in situ video recording <i>National Technical University "Kharkiv Polytechnic Institute", Kharkiv, Ukraine</i>
16:20-16:40	Session: Biomaterials Keynote talk Dr. Pankaj Bharmoria (I23) Recyclable Photon Upconversion Crystals Doped Bacterial Cellulose Composite Films for Sustainable Photonics <i>Barcelona Materials Science Institute (ICMAB-CSIC), Barcelona, Spain</i>
16:40-17:00	Session: Micro / Nano Materials Keynote talk Dr. Pavel Zelenovskii (I4) Unusual water dynamics in peptide nanochannels <i>Department of Chemistry & CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal</i>
17:00-17:15	Session: Biomaterials Prof. Dr. Alessandra Maria Bossi (O20) Biocompatible biomimetics made by the molecular imprinting of silk fibroin <i>University of Verona, Dept. of Biotechnology, Strada Le Grazie 15, 37134 Verona, Italy</i>



17:15-17:30	Session: New Energy Materials Prof. Dr. Aliru Olajide Mustapha (O16) Nano-Calcium Oxide (n-CaO) from Various Waste Bones and Cooking Oils in the Production of Biodiesel: Catalytic Performance <i>Department of Chemistry and Industrial Chemistry, Faculty of Pure and Applied Sciences, PMB 1530, Ilorin, Kwara State, Nigeria</i>
17:30-17:45	Session: Nanotechnology Duarte Almeida (O19) Multiphasic delivery nanosystems for delivery of Li-doped albumin nanoparticles for neutron capture therapy <i>TEMA – Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal</i>
17:45-18:00	Session: Biomaterials Keynote talk Dr. Alejandro Heredia Barbero (I13) Infrared spectroscopy and atomic force microscope as nanotechnological tools for amino acid chemical evolution and prebiotic chemistry <i>Departamento de Química de Radiaciones y Radioquímica, Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, Mexico</i>
18:00-18:30	Conference Closing Ceremony



Poster session, July 11, 2024 (Thursday), 16:00-18:30

P1	Numerical study of the mechanical behaviour of concrete with polypropylene fibre SAHNOUN ILHEM, GUEMMADI Z, TOUMI B <i>MCB, Materials and Sustainability Laboratory (LMDC), Route Ain El bey, Constantine, Algeria</i>
P2	Photodegradation of Methylene Blue by CeO₂/NiO Modified Silicon Nanowires Afaf Brik, Sabrina Naama, Karima Benfadel, Toufik hadjersi, Seif eddine friha <i>Research Centre of semi-conductor Technology for Energy, CRTSE-02, Bd.Dr.Frantz FANON, B.P.140 Algiers-7, Merveilles, 16038, Algeria</i>
P3	Photoelectrochemical Conversion of CO₂ using HCl-PANI/Cu Photocathode Lamia Talbi, Karima Benfadel, Sabiha Anas Boussaa, Samira Kaci, Assia Boukezzata, Yahia Ouadah <i>Research Center on Semiconductor Technology for Energetic, Division TESE-CRTSE, 2BD Frantz Fanon, P B 140, 7 Merveilles, Algiers, Algeria</i>
P4	Impact of silicon surface modification on the catalytic performance towards CO₂ conversion of Cu₂S/Si-based photocathodes Karima Benfadel, Lamia Talbi, Sabiha Anas Boussaa, Afaf Brik, Assia Boukezzata, Yahia Ouadah, and Samira Kaci <i>Research Center on Semiconductor Technology for Energetic, Division TESE-CRTSE, 2BD Frantz Fanon, P B 140, 7 Merveilles, Algiers, Algeria</i>
P5	The Properties of lightweight artificial aggregates from construction waste Katarzyna Kalinowska-Wichrowska, Edyta Pawluczuk, Michał Bołtryk, Małgorzata Franus, Adam Masłoń <i>Białystok University of Technology, Białystok, Poland; Lublin University of Technology, Lublin, Poland; Rzeszów University of Technology, Rzeszów, Poland</i>
P6	A biocompatible acrylic resin with solvent as a potential material for obtaining microneedle transdermal systems using masked stereolithography Dorota Tomczak, Wiesław Kuczek, Ariadna B. Nowicka, Tomasz Osmałek, Monika Wojtyłko, Radosław Wichniarek <i>Institute of Chemical Technology and Engineering, Poznań University of Technology, Berdychowo 4, 60-965 Poznań, Poland; Faculty of Mechanical Engineering, Poznań University of Technology, Piotrowo 3, 61-138 Poznań, Poland; Faculty of Materials Engineering and Technical Physics, Poznań University of Technology, Piotrowo 3, 60-965 Poznań, Poland; Chair and Department of Pharmaceutical Technology, Poznań University of Medical Sciences, Rokietnicka 3, 60-806 Poznań, Poland</i>



P7	The Properties of cement composites with lightweight artificial aggregates produced from construction and industrial waste Edyta Pawluczuk, Katarzyna Kalinowska-Wichrowska, Marta Kosior-Kazberuk, Małgorzata Franus, Adam Mastoń <i>Białystok University of Technology, Białystok, Poland; Lublin University of Technology, Lublin, Poland; Rzeszów University of Technology, Rzeszów, Poland</i>
P8	Preparation and characterization of Al alloys modified by the addition of Re for Spark Plasma Sintering Alicja Duda, Krzysztof Pęczak, Piotr Tomczyk, Grzegorz Matula, Adriana Wrona <i>Łukasiewicz Research Network – Institute of Non-Ferrous Metals, Sowinskiego 5 St. 44-100 Gliwice, Poland; Doctoral School, Silesian University of Technology, Akademicka 2A St., 44-100 Gliwice, Poland; Nanotechnology and Materials Technology Scientific and Didactic Laboratory, Faculty of Mechanical Engineering, Silesian University of Technology, Towarowa 7A St., 44-100 Gliwice, Poland</i>
p9	Application of semiconductor-based APS coatings for the light-activated decomposition of persistent organic pollutants Alicja Duda, Bartosz Kopyciński, Łukasz Hawełek, Krzysztof Pęczak, Piotr Tomczyk, Grzegorz Muzia, Adriana Wrona <i>Łukasiewicz Research Network – Institute of Non-Ferrous Metals, Sowińskiego 5 St., 44-100 Gliwice, Poland; Łukasiewicz Research Network – Institute for Engineering of Polymer Materials and Dyes, Marii Skłodowskiej-Curie 55 St., 87-100 Toruń, Poland; Doctoral School, Silesian University of Technology, Akademicka 2A St., 44-100 Gliwice, Poland</i>
P10	Physical and mechanical properties of mortars with synthetic zeolites Wojciech Franus <i>Lublin University of Technology, Lublin, Poland</i>
P11	Influence of firing temperature on the properties of eco-friendly lightweight aggregates Małgorzata Franus, Danuta Barnat-Hunek, Rafał Panek, Katarzyna Kalinowska-Wichrowska, Edyta Pawluczuk, Adam Mastoń <i>Lublin University of Technology, Faculty of Civil Engineering and Architecture, Nadbystrzycka 40 Street, 20-618, Lublin, Poland; Białystok University of Technology, Faculty of Civil Engineering and Environmental Sciences, Wiejska 45 E Street, 15-351 Białystok, Poland; Rzeszów University of Technology, Faculty of Construction, Environmental Engineering and Architecture. Al. Powstańców Warszawy 6 Street, 35-959 Rzeszów, Poland</i>
P12	Influence of low-silicon and high-silicon zeolite addition on changes in the microstructure of pastes Joanna Styczen <i>Lublin University of Technology, Lublin, Poland</i>



P13	Rejuvenating agents of waste origin used in the mix asphalt with RAP Agnieszka Woszuik, Wojciech Franus <i>Lublin University of Technology, Faculty of Civil Engineering and Architecture, Department Geotechnical Engineering, Nadbystrzycka 40, 20-618 Lublin, Poland</i>
P14	Study of the antibacterial effect of fluorohydroxyapatite combined with ginger oil extract Maissa AGSOUS, Hafit KHIREDINE, Sabeha YALA <i>Faculty of Technology, University of Bejaia, Targa Ouzemour, Algeria</i>
P15	Multiscale studies of electric micropropulsion for small spacecraft Manish Jugroot, Cecile Malardier-Jugroot <i>Mechanical and Aerospace Engineering, Royal Military College of Canada, Kingston, ON, Canada; Chemistry and Chemical Engineering, Royal Military College of Canada, Kingston, ON, Canada</i>
P16	Tunable Raman features in nanomaterials belonging to Nb₂O₅-SiO₂, binary oxide systems Luigi Sirleto, Claudio Imparato, Aurelio Bifulco, Paola Amato, Antonio Aronne, Alessandro Vergara <i>National Research Council, Institute of Applied Sciences and Intelligent Systems, Naples, Italy; Dept. of Chemical, Materials and Production Eng., University of Naples Federico II, Naples, Italy; National Interuniversity Consortium of Materials Science and Technology, Florence, Italy; Dept. of Chemical Science, University of Naples Federico II, Naples, Italy</i>
P17	Statistical Tolerance Synthesis based on Jacobian Torsor Model and form deviations in mechanical assemblies Said Boutahari, Mustapha El Mouden, Mouhssine Chahbouni <i>TSI laboratory, Higher school of technology, Sidi Mohammed Ben Abdellah University, Imouzzet street, BP 2626 (30000), Fez, Morocco</i>
P18	Anelasticity, internal friction in radiation and structural functionalized nanocomposites of multiwalled carbon nanotubes and polyamide, polyethylene, polyvinylchloride, SiO₂ A.P. Onanko, D.V. Charnyi, Y.A. Onanko, O.P. Dmytrenko, M.P. Kulish, T.M. Pinchuk-Rugal, M.V. Yatsiuk, E.M. Matselyuk, V.M. Popruzhenko, O.L. Pavlenko, T.O. Busko, A.M. Gaponov, L.I. Kurochka, P.P. Ilyin, S.V. Marysyk <i>Kyiv national university, Kyiv, Ukraine</i>
P19	Local electromechanical properties of Glycine-Diphenylalanine tubes composites Igor Bdikin <i>TEMA: Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal; LASI—Intelligent Systems Associate Laboratory, Guimarães, Portugal</i>



P20	Development of thermoelectric composites with catalytic functionality Miguel A.Vieira, Andrei Kovalevsky, Aleksey Yaremchenko <i>CICECO – Aveiro Institute of Materials, Department of Materials Engineering and Ceramics (DEMaC), University of Aveiro, 3810-193, Aveiro, Portugal</i>
P21	Effect of mechanical recycling on structural, mechanical and optical properties of high-density polyethylene (HDPE) Raul Simões, J. Rodrigues, Teresa Monteiro, Victor Neto and Gil Gonçalves <i>Department of Mechanical Engineering; Centre for Mechanical Technology and Automation; University of Aveiro, Portugal; i3N, Department of Physics, University of Aveiro, Portugal; LASI - Intelligent Systems Associate Laboratory, 4800-058 Guimarães, Portugal</i>
P22	Two-dimensional conductive cobalt metal-organic frameworks for high performance supercapacitors Shashank Sundriyal, Aristides Bakandritsos <i>Regional Center of Advanced Technologies and Materials, The Czech Advanced Technology and Research Institute (CATRIN), Palacký University Olomouc, Šlechtitelů 27, 779 00 Olomouc, Czech Republic</i>
P23	Microwave activated mixed biowastes derived porous carbon-based electrode for all-solid-state symmetrical supercapacitors Vishal Shrivastav, Wojciech Nogala <i>Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland</i>
P24	Porphyrin – Based Carbon Dots for Photodynamic Therapy Mariana Dias, Carla Santos, Gil Gonçalves <i>Centre for Mechanical Technology and Automation (TEMA), Mechanical Engineering Department, University of Aveiro, 3810-193 Aveiro, Portugal; Intelligent Systems Associate Laboratory (LASI), 4800-058 Guimarães, Portugal; CQE, Centro de Química Estrutural, Instituto Superior Técnico, Av. Rovisco Pais, 1049-001 Lisboa, Portugal; LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal</i>
P25	Enhanced Supercapacitor Performance with Redox Additive Electrolytes for UiO-66@ZIF-8 Material Study Mansi, Vishal Shrivastav, Shashank Sundriyal, Umesh Kumar Tiwari <i>CSIR-Central Scientific Instrument Organisation (CSIR-CSIO), Chandigarh 160030, India; Academy of Scientific and Innovative Research, Ghaziabad, 201002, India; Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland; Regional Center of Advanced Technologies and Materials, The Czech Advanced Technology and Research Institute (CATRIN), Palacký University Olomouc, Šlechtitelů 27, 779 00 Olomouc, Czech Republic</i>



P26	Development of Green Carbon Dots and Metal Frameworks based nanocomposites for Printable Biosensors Disha, Wojciech Nogala <i>Institute of Physical Chemistry Polish Academy of Sciences (IChF), Warsaw, Poland</i>
P27	Comparison of local surface properties of copper and mild steel under corrosion Jessica Cardoso, Igor Bdikin, Ricardo Beja, António Pereira <i>TEMA: Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal; LASI—Intelligent Systems Associate Laboratory, Guimarães, Portugal</i>
P28	Polymeric Nanoparticles for Drug Delivery, using Bovine Serum Albumin for Prostate Cancer Treatment: An In Vitro Study Beatriz Teixeira, Sónia A.O. Santos, Mónica Almeida, Miguel Oliveira, Ricardo J.B Pinto <i>Department of Biology University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal; Aveiro Institute of Materials (CICECO), Department of Chemistry – University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal; Centre for Environmental and Marine Studies (CESAM), Department of Biology University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal</i>
P29	Sensitizing effect of Yb3+ ions on 1.53 μm broadband and 548nm upconversion green emissions of Er3+-doped TeO2–WO3–GeO2 glasses B.C. Jamalaiaha, Sk.Nayab Rasoola, K. Venkata Raob, M.J. Soaresc, G. Viswanadhaa, K. Pavani <i>Department of Physics, Rajeev Gandhi Memorial College of Engineering and Technology (Autonomous), Nandyal, Andhra Pradesh 518501, India; Department of Physics, Government Degree College, Porumamilla, Andhra Pradesh 516193, India; Department of Physics, I3N, University of Aveiro, Aveiro 3810-193, Portugal</i>
P30	Experimental study of electron beam welding parameters for joining copper pipes in heat pumps Sathishkumar Duraisamy, João Dias, Antonio Bastos, Ana Horovistiz <i>TEMA, Department of Mechanical Engineering, University of Aveiro, Portugal</i>



Plenary lectures



The origin of the low-temperature resistivity upturn in strontium ferromolybdate ceramics

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In this work, we propose a novel explanation of the low-temperature resistivity minimum in ceramic strontium ferromolybdate that shows better agreement with given experimental data from various publications [1]. We demonstrate that in SFMO ceramics, SFMO thin films deposited by pulsed laser deposition including (100) and (111) textured thin films, as well as in nonstoichiometric SFMO ceramics, an intergrain tunneling mechanism of charge carrier conduction leads to a decrease in resistivity with increasing temperature in the low-temperature region. This intergrain tunneling can be attributed to fluctuation-induced tunneling. On the other hand, bulk metallic resistivity of the grains, which increases with temperature, becomes dominant at higher temperatures and magnetic fluxes. The interplay of these conduction mechanisms leads to a resistivity minimum, i.e., a resistivity upturn below the temperature of minimum resistivity. Several mechanisms have been discussed in the literature to describe the low-temperature upturn in resistivity. According to our findings, the resistivity upturn is not caused by a semiconductor-metallic transition, but it can be attributed to intergrain fluctuation-induced tunneling limiting the metallic bulk conductivity of SFMO grains in the absence of a magnetic field or at low values of its flux density as well as at low temperatures.

Additionally, we obtained that in the region of metallic conductivity at higher temperatures and magnetic fluxes, the pre-factor R_m of the temperature-dependent term of metallic conductivity written as a power law decreases exponentially with the temperature exponent m of this power law. Here, the value of m is determined by the charge scattering mechanism.

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Sustainable Approaches for Printable Sensors and Actuators

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The rapid digitalization of the society and the economy, associated to concepts like Internet of Things and Industry 4.0 is boosting the increasing implementation of sensors and actuators. Printing technologies are called to play a major role in this field, as it allows the necessary steps towards sustainable digitalization.

In this talk the relevance, formulations, types, and applications of sustainable inks and substrates for sensors and actuators will be addressed. Applications ranging from temperature, deformation and humidity sensors will be shown, together with bending actuators for soft robotic applications, among others.



Emerging sensing Approach for health and Environmental management

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Presently nano-enabled smart sensing technology interfaced with other tools like the Internet of Things (IoT) and artificial intelligence (AI) are emerging significantly for efficient disease/problem management, even at point-of-care (POC) applications. Such systems are on the track of transformative research according to the goals of 5th and 6th-generation technology to track and manage health and the environment according to sustainability goals. In this direction, we are exploring electro-active electrodes for efficient bio (biosensor) and chemical sensing with the capability of POC applications. Our developed sensing prototypes are well interfaced with a miniaturized potentiostat (M-P) which can be operated using a smartphone. To develop efficient infectious disease management, we have recently developed miniaturized nano-enabled biosensing systems to detect targeted biomarkers for diagnostics of infectious diseases like COVID-19 infection. Further, electrochemical sensing is explored for efficient sensing of water pollutants (heavy metals) and forever chemicals like microplastics selectively and at a very low level (ppm to ppb). We believe our developed biosensing and chemical sensing systems supported by AI and IoT approaches can be a potential tool for personalized health management and environment surveillance. The outcomes of these sensing technologies can be utilized for policy and timely decision-making efforts.



Supported catalysts for CO₂ cycloaddition reactions

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One of the main greenhouse gases (GHGs) that humans are releasing into the atmosphere as a result of increased activity is carbon dioxide (CO₂).

On the other hand, cyclic carbonates are valuable compounds that serve a variety of purposes in chemical synthesis, including as an intermediate and polar aprotic solvent. The cycloaddition reaction of CO₂ and epoxides was found to be a promising method for the synthesis of cyclic carbonates, because it uses CO₂ as a feed stock, contributing to the reduction of CO₂ in the environment.

In the current study, graphene oxide (GO) was synthesized using Tour's method and functionalized with different amine groups including. The as-synthesized functionalized GO catalysts were characterized using various techniques which confirmed the successful functionalization of the various amine groups on the GO.

The synthesis of styrene carbonate (SC) from CO₂ and styrene oxide (SO) using the as-synthesized catalysts was selected as the model reaction in order to investigate the influence of the reaction conditions (temperature, catalyst amount, solvent and reaction time) on the catalytic activity of the catalyst, and to determine the optimum reaction conditions.

The catalytic activity of all the as-synthesized amine-functionalized GO was studied in the cycloaddition of CO₂ with other epoxides, namely, epichlorohydrin (EPC) and propylene oxide (PO) for the synthesis of 3-chloropropylene carbonate (CPC) and propylene carbonate (PC), respectively.

Quaternary ammonium salts grafted GO were synthesized in an attempt to study and enhance the catalytic activity.

The catalyst recyclability was also investigated using GO-APTES where it was found that the catalyst could be reused three times without significant loss of catalytic activity.

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Invited speakers



11. Development of Biopolymer-Based Hydrogels with Varying Porosity Ratio

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Hydrogels are materials that attract the attention of researchers around the world and have a wide range of applications such as solar cells, smart systems, wound dressings, shape-memory materials and biomedical applications [1-4]. In our study, we develop polyvinyl alcohol (PVA)-based hydrogels with different amounts of carboxymethyl cellulose (CMC). A three-dimensional hydrogel matrix was achieved using a non-toxic cross-linker. This hydrogel matrix was supported by the freeze-thaw method, another non-toxic cross-linking technique. The prepared biopolymer-based hydrogels' changing porosity ratio and pore size were visualized with a field emission scanning electron microscope, and the images were analyzed with ImageJ software. The software shows that PVA/CMC(100:50) hydrogel has a porosity of 45.48% and pore sizes ranging from 2.714-69.16 μm . PVA/CMC(100:75) hydrogel has 63.722% porosity and pore sizes ranging from 2.244-73.54 μm . PVA/CMC(100:100) hydrogel has a porosity of 42.53% and pore sizes ranging from 3.429-32.62 μm . In conclusion, it was observed that the CMC additive in the prepared biopolymer-based hydrogels changed the hydrogels' porosity ratio and pore size.

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I2. Synthesis, Characterization and Photocatalytic applications of New Composite system

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SnO₂ nanoparticle were synthesized Hydrothermal reaction method using stannous chloride dehydrate (SnCl₂·2H₂O), (NH₄OH). SnO₂ nanoparticle were characterised by XRD, IR, UV, FESEM. XRD results spectrum display mainly oxygen and Tin peaks, which indicates tin as tetragonal rutile structure and average crystalline size of 4.5nm. FESEM micrographs shows that synthesized SnO₂ has flower-like structure. The obtained SnO₂ particle are homogenous and consist in size which corresponds to the XRD results that exhibit good crystallinity. This paper demonstrates the synthesis of SnO₂ nanoparticle using Hydrothermal reaction method. By using cyclohexanedione and ortho-phthaldehyde as substrate 6,13 pentacenequinone and SnO₂ were opted nanocomposite because of their optical properties, Band gap which is 3.6ev and 3.37ev respectively, thermal stability and photo catalytic activity. Crystal violet dye is degraded at higher rate using coupled semiconductor PQ/SnO₂ than individual PQ and SnO₂, concluding the higher degradation rate for high % PQ than lower. The proposed method can also be used for synthesizing other semiconductor PQ containing nanoparticle.



I3. Sustainable thermoelectrics: the potential of strontium titanate

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Thermoelectric technology is pivotal for a sustainable future, providing a solution to one of the most persistent challenges of modern society: energy efficiency. By directly converting heat into electricity, thermoelectric generators enable the recovery of energy that would otherwise dissipate uselessly into the environment. Oxide materials, composed of naturally abundant, non-toxic elements, are recognised as a viable alternative to conventional thermoelectrics. They offer the capability to operate at elevated temperatures, which leads to enhanced Carnot efficiency, and exhibit remarkable structural and microstructural versatility. Strontium titanate emerged as a front-runner among n-type oxide thermoelectrics owing to its promising electronic properties, phase stability, and exceptional flexibility for tuning by substitution and incorporating A-site and oxygen deficiency. In addition, strontium titanate is chemically compatible with many other materials, enabling a variety of thermoelectric composite approaches. A concise overview of the underlying mechanisms responsible for promising thermoelectric performance will be presented, together with current trends in the design of thermoelectric materials based on strontium titanate.



I4. Unusual water dynamics in peptide nanochannels

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It is well known that physical properties of water confined in nanochannels essentially differ from a macroscopic bulk state. Ionic functional groups, covering internal surface of peptide nanochannels, can modify water organization and behavior and additionally bias its properties. Therefore, the study of such systems is of great fundamental and practical importance. In this work, we analyzed the structure and dynamic behavior of water confined in nanotubes made of several dipeptides: dileucine (Leu-Leu, LL), alanine-valine (Ala-Val, AV), tryptophan-glycine (Trp-Gly, WG), and diphenylalanine (Phe-Phe, FF). The peptide shell configuration arranges the water molecules in linear chains, single and double spirals. The analysis of solid-state NMR spectra, DFT calculations, and molecular dynamics simulation revealed several types of water molecules in the nanochannels differ in their dynamics and the diffusion character. Dynamic vapor sorption measurements were used to derive their self-diffusion coefficients. The obtained results demonstrate a great potential for peptide nanotubes use for transportation of small molecules and ions, such as lithium, in energy storage devices and micro- and nanofluidic systems.

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I5. Cellular Metals in Engineering Applications

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Cellular metals have emerged as paramount lightweight, multifunctional materials, driving significant progress within various industrial sectors. Their attributes—lightweight, robust, multi-functional, recyclable, and non-flammable—make them ideal for sustainable design. This presentation provides a comprehensive overview of research activities in the field of cellular metals [1-4], focusing on design, processing, and morphological and mechanical characterization of structures filled with various cellular metal cores (e.g. open-cell aluminium foam, closed-cell aluminium foam, advanced pore morphology foam, metallic hollow sphere structure). The structures undergo mechanical testing under various loading conditions, revealing insights into deformation responses, collapse mechanisms, and mechanical properties. Results indicate the potential for tailored mechanical properties, aligning with specific applications, showcasing the versatility and performance of filled cellular structures.

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I6. Photoluminescent Active Ion-Doped Glasses for Advanced Gas Sensing Applications

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Glasses doped with photoluminescent (PL) active ions, specially trivalent rare earth (RE^{3+}) ions offer significant advancements in gas sensing due to their enhanced optical properties and high sensitivity. This presentation is on various glass matrices, including silica, phosphate, tellurite, and chalcogenide, doped with ions like europium (Eu^{3+}), erbium (Er^{3+}), and ytterbium (Yb^{3+}). These dopants impart distinct PL characteristics, enabling gas detection across visible (VIS), infrared (IR), and mid-infrared (MIR) regions.

Eu^{3+} -doped glasses, which emit sharply in the VIS around 615 nm, are ideal for detecting oxygen (O_2), as O_2 presence quenches PL intensity. Er^{3+} -doped glasses are effective in the IR region around 1.5 μm , suitable for carbon dioxide (CO_2) detection, with PL intensity correlating to CO_2 concentration. Yb^{3+} -doped tellurite glasses, emitting strongly in the MIR around 1 μm , are effective for sulfur dioxide (SO_2) detection, enhancing sensitivity and selectivity. Chalcogenide glasses doped with Er^{3+} and Yb^{3+} show potential for methane (CH_4) detection due to their broad MIR transmission and high refractive index. These glasses are fabricated into optical fibers, which detect gases through changes in PL emission upon exposure. This method allows remote sensing, high sensitivity, and operation in harsh environments, making it suitable for environmental monitoring and industrial applications.

The presentation will include a general introduction to glasses and their properties, an overview of PL through various dopants, and a discussion on different PL mechanisms. It will also cover the fabrication of glasses and fibers, especially chalcogenide glasses, and detail the mechanisms of gas detection using these advanced materials.



17. Enhancement in ultraviolet photodetection of DyCrO₃/n-Si heterojunction devices with manganese substitution

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Ultraviolet (UV) radiation is a part of electromagnetic radiation that impacts human life. It is classified into three bands, from 320 to 400 nm as UVA, 280 to 320 nm as UVB, and 100-280 nm as UVC, according to the International Commission on Illumination's standard. The interaction of UVB radiation with the stratum corneum produces 90% of the vitamin D required by the human body, which aids in healthy bone formation. However, exposure to high levels of UVB light accelerates the ageing process and even causes the skin cancer in humans. Therefore, there is an urgent need for advancements in UV photodetectors. Broadband semiconductors, especially metal oxides, are commonly employed in UV photodetectors. Amongst the metal oxides, DyCrO₃ compound distinguishes itself as a prominent wide bandgap semiconductor, featuring a significant bandgap energy spanning from 2.8 to 3.1 eV. The semiconducting nature of this material makes it an ideal material for UV photodetectors.

We investigated the influence of manganese (Mn) substitution on the photoelectrical properties of spin coated DyCr_{1-x}Mn_xCrO₃ ($x = 0, 0.20, 0.50$) thin films deposited on n-type Si substrate. The current-voltage (I - V) characteristics of the fabricated devices exhibited the diode behaviour. I - V behaviour of the films followed the trap assisted tunneling (TAT) and space-charge-limited conduction (SCLC) conduction mechanisms at higher and lower fields, respectively. Transient photocurrent measurements were performed on the fabricated films when the films were exposed to ultraviolet light of wavelengths 365 and 254 nm and an on/off cycle of 20 sec. It was observed that the photosensitivity was 142%, 233% and 429% for DyCrO₃ (DCO), DyCr_{0.8}Mn_{0.2}CrO₃ (DCMO20), and DyCr_{0.5}Mn_{0.5}O₃ (DCMO50) heterojunction devices, respectively. These devices also exhibited a significant increase in responsivity, ranging from 7.81×10^{-4} mA/W to 1.01831 mA/W, corresponding to a concentration increase of Mn from 0 to 50%. From these measurements, various device essential metrics such as sensitivity, responsivity, detectivity, quantum efficiency and linear dynamic response were determined. In conclusion, the Mn substitution was found to significantly enhance the UV detection of DyCrO₃/n-Si heterojunction devices.



I8. Non-concentration quenching phenomena in red-emitting Eu^{3+} doped layered bismuth tungstate Aurivillius family compound

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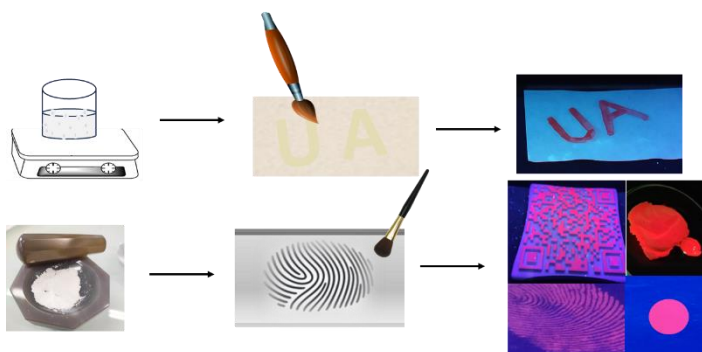
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Abstract: Layered arrangement of Aurivillius compounds supports the non-concentration quenching phenomenon even with high concentrations of Eu^{3+} ions as dopants. The developed Eu^{3+} doped phosphors of such a kind are tested in various applications such as latent fingerprint detection and flexible screen-printing polymers.

Introduction: The alternative stacking of $(\text{RE}/\text{Bi}_{2-x}\text{O}_2)^{2+}$ and $(\text{WO}_4)^{2-}$ ion layers accept the high concentrations of dopant $x\text{RE}^{3+}$ ions in the A-site (Bi^{3+}), leading to the promotion of tunable band gap structure and optical properties. Energy migration phenomenon which is more prominent in Eu^{3+} doped compounds can be controlled through Aurivillius type of compounds.

Methods: Solid state reaction method, X-ray diffraction (XRD), Raman spectroscopy, Fourier Transform Infra-red (FT-IR ATR), Diffuse Reflectance Spectroscopy (DRS), Scanning Electron Microscopy (FE-SEM-EDX), TEM, XPS, Photoluminescence, J-O theory.



Results / Discussion: The present compounds are iso-structural to the high-temperature phase (HT) of Bi_2WO_6 . Absorption results confirm the broad LMCT band (200-475nm) and sharp transitions, attributed to La-O CTB, Bi^{3+} ($^1\text{S}_0 \rightarrow ^3\text{P}_1$) and Eu^{3+} f-f transitions (380-570 nm). Under near-UV excitation the optimized Eu^{3+} doped compound emits a bright intense red emission (612 nm) with CIE coordinates of (0.64,0.36), color purity of 93 %. Thermal stability was tested in the temperature range of 30-150°C. The as-synthesized compounds were tested in various polymers for luminescent inks.

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19. Mixed ionic and electronic conductors for Solid Oxide Cells

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Mixed ionic and electronic conductors (MIECs) have garnered increased attention due to their potential to enhance the performance of solid oxide cells (SOCs) applications, including solid oxide fuel cells (SOFCs) and solid oxide electrolysis cells (SOECs) [1]. This work presents a comprehensive study on the fabrication, characterization, and performance evaluation of different MIEC compositions as air electrodes. Emphasis is placed on their electrochemical properties, *i.e.*, oxygen reduction reaction (ORR) kinetics under various operational conditions. Advanced characterization techniques, such as X-ray diffraction (XRD), scanning electron microscopy (SEM), and electrochemical impedance spectroscopy (EIS), are employed to elucidate the relationship between microstructure and electrochemical performance. The implications of these findings for the design of next-generation SOC are discussed, highlighting the critical role of MIECs in advancing sustainable energy technologies.

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110. Effect of ion implantation in alkali borate glasses

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Alkali borate (ABO) glasses of the composition ($20A_2O-80B_2O_3$, where A= Li, Na and K) were prepared using the thermal melt quenching technique. Pure analytical grade chemicals boric acid (H_3BO_3), lithium carbonate (Li_2CO_3), sodium carbonate (Na_2CO_3) and potassium carbonate (K_2CO_3) from Sigma Aldrich >99.99% were used as reactants. The effect of He^+ ion implantation on the structural, optical properties and refractive index of the ABO glasses prepared by melt quenching was investigated. SRIM and TRIM simulation tools were used to understand certain ion dependent parameters like depth, kurtosis, straggle and skewness for He^+ ion implantation at 100 keV on the ABO glasses [1]. Density and its related structural parameters like molar volume, molar volume of oxygen, oxygen packing density, boron – boron separation and bond density were also calculated [2]. XRD shows the unaltered amorphous nature of lithium and sodium borate glasses even after implantation. KBO glasses possess polycrystalline behaviour when subjected to ion implantation due to ceramization of the glasses. These polycrystalline KBO glasses are matched with Potassium Dihydrogen Dioxonium Decaoxopentaborate of orthorhombic structure. The E_g decreases under He^+ ion implantation in all the prepared glasses after irradiation. The change in refractive index was found using metricon prism coupler for pristine and implanted samples. The change in refractive index implies the implanted glasses are very suitable for optical waveguides.

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I11. Shape Optimization for Broadband Vibration-based Piezoelectric Energy Harvesters

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Broadband vibration-based piezoelectric energy harvesters (PEHs) have emerged as a promising technology for converting ambient mechanical vibrations into electrical energy, suitable for powering small-scale electronic devices. Shape optimization plays a crucial role in enhancing the performance of broadband vibration-based PEHs. Shape optimization is very effective to maximize the harvested energy as well as to broaden the working frequency range by modifying the geometrical design of the harvester. This paper reviews the design and optimization of PEHs to achieve efficient energy harvesting across a wide range of vibration frequencies. By analyzing various structural configurations and shape topology, we aim to identify key factors that influence the broadband performance of these devices. This study provides valuable insights into the design of more effective energy harvesters, paving the way for their wider application in diverse environments where energy harvesting from ambient vibrations is desirable.



I12. Low-Voltage Scanning Electron Microscopy as a Crucial Tool for Optimizing the Properties of Polymer-Nanoclay Composites

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Introduction: Field-Emission Gun Scanning Electron Microscopes such as the NovaSEM are a powerful tool in nanocomposites studies because they provides images with high resolution up to few nanometers at a high magnification. An electron beam with low loading energy (2.2 KeV) was used to reduced specimen surface charging and damage. In addition two different detectors were used for imaging the samples; a Through-lens-detector (TLD) for secondary electron imaging at low magnification and concentric back scatter detector (CBS) using back-scattered electrons to obtain high magnification images. CBS was found the most valuable tool for the challenging task of studying Polymers/clay interfaces. CBS in conjunction with beam deceleration is used to map nanoclay distribution on polymer particles [1].

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

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

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I13. Infrared spectroscopy and atomic force microscope as nanotechnological tools for amino acid chemical evolution and prebiotic chemistry

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Chemical evolution is the change of molecular compounds towards their increase in complexity and functionality. At the nanoscale, the analysis has been greatly facilitated by the use of infrared spectroscopy (FTIR) and atomic force microscopy (AFM) to understand the changes in molecules interacting with specific prebiotic conditions. By utilizing these powerful tools, we are able to investigate the behavior of amino acids at the molecular level within crystalline structures towards the polymerization to form possible molecular dynamic oligomers. One of the key areas of interest in this field is understanding the formation and evolution of amino acid crystals and the formation of oligomers with possible catalytic properties. Amino acids are organic molecules that form proteins and as such might have been of relevance in prebiotic chemistry and molecular evolution. In this work, we show the relevance to visualize these molecules with the AFM and FTIR providing valuable insights into their behavior within crystal formations possessing hydrogen bonds and more complex oligomers with peptide bonds. These are processes that drive the chemical evolution of these structures. One of the key advantages of using these nanotechnological tools is to have images and some emerging properties from the peptide bonds (FTIR), phase images and indentations (AFM) from the molecular interactions.

By studying the chemical evolution of amino acids at the nanoscale using FTIR and AFM, we are gaining important insights into the origins of chirality and other processes that drive prebiological chemical evolution. This research has the potential to impact the possible formation of chiral oligomers of amino acids. In conclusion, the use of nanotechnological methods (atomic force microscopy and FTIR) to study the chemical evolution of amino acids from crystals to oligomers has opened new opportunities to explore molecular evolution under controlled experiments. This research is in progress in our group.

Financial support: UNAM-DGAPA-PAPIIT IN205522

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I14. Electrospray alloying and Electrochemical Methods as Effective Technologies for Obtaining Advanced Materials

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Among various surface modification technologies, such as physical vapor deposition, magnetron plasma sputtering, plasma-electrolytic saturation of the surface, etc., electrospray alloying (ESA) or electrospray deposition (ESD) conquers a distinct place due to the following advantages: (1) a wide range of materials which can be used as alloying elements and the possibility to obtain multicomponent coatings and control their properties; (2) strong metallurgical bonds between the modified surface and the substrate; (3) high corrosion and wear resistance of obtained materials. This method is based on the transfer of anode material to the treated surface by spark discharges in various environments: air, inert gas, dielectric liquid, etc., and vacuum.

On the other hand, electrochemical methods are used to synthesize a large number of compounds and materials with versatile applications. The shape, size, and dimensions of the material can be easily controlled by using either template-assisted or template-free electrochemical methods. Some advantages of electrochemical synthesis are (1) a large redox potential range accessible by selecting an appropriate combination of electrode materials, solvents, and supporting electrolytes. (2) precise control over materials composition and current efficiency due to precise choice of potential and current, (3) deposition in deep recesses.

This presentation is dedicated to the celebration of 60 years of establishing the Institute of Applied Physics and will overview the experience gained in the obtaining of new and advanced materials.

Acknowledgment. The author gratefully acknowledges the colleagues' contribution and support from MSCA grant №778357- SMARTELECTRODES, and the ANCD project 011204.



I15. Crystallization modes in amorphous films of V_2VI_3 semiconductors according to TEM with *in situ* video recording

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Amorphous films of Sb_2S_3 and Sb_2Se_3 with layer thicknesses $h = 25\text{--}40\text{ nm}$ were grown on KCl single crystals at room temperature by thermal evaporation in vacuum. Electron-beam crystallization of films was studied by the methods of transmission electron microscopy "in situ" with video registration of structural changes.

It was revealed, that Sb_2S_3 films of stoichiometric composition crystallize polymorphous in a single stage (Fig. 1). Films with the excess of Sb crystallize in two stages [1]. There is predominant crystallization of Sb during the first stage of the process, and subsequent crystallization of matrix of Sb_2S_3 during the second stage (Fig. 2).

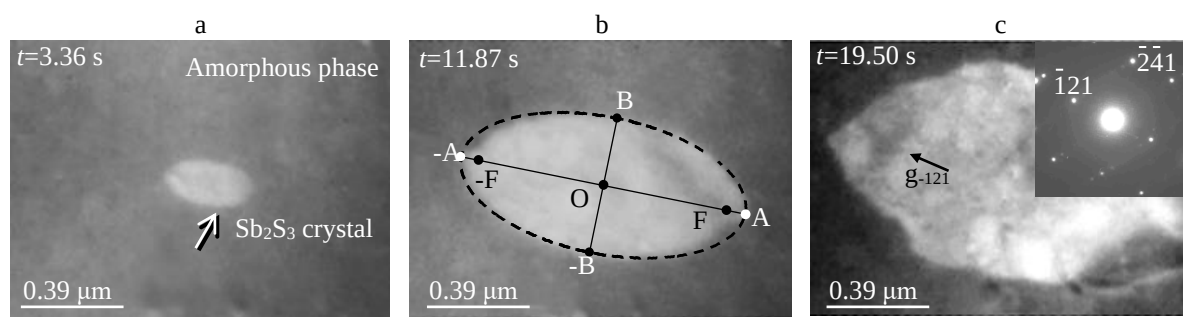


Fig. 1. Polymorphous crystallization of amorphous film of Sb_2S_3 . Time moments t , that has passed from the beginning of the recording, are shown in the upper corner of each frame. SAED pattern of the crystalline Sb_2S_3 is shown in the upper right corner of the frame 1c. The dotted line marks the ellipse with eccentricity 0.881

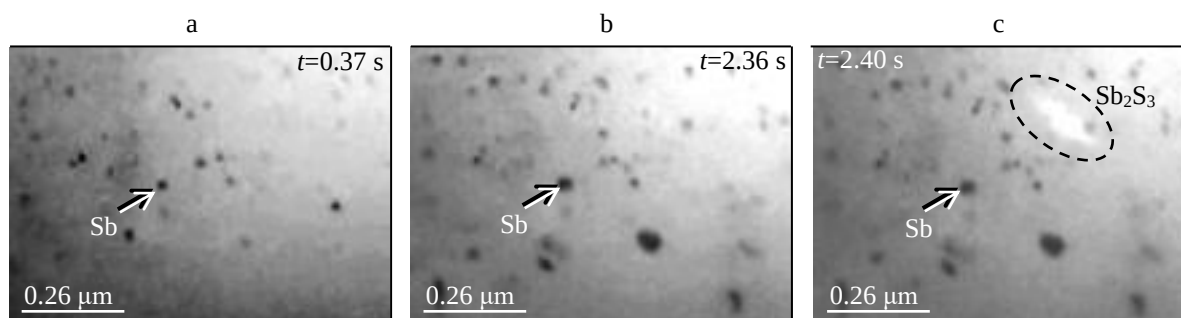


Fig. 2. Primary crystallization of Sb in amorphous film. Time moments t that has passed from the beginning of the recording are shown in the upper corner of each frame. The moment of the appearance of Sb_2S_3 crystal is fixed in the upper corner of the frame 4c

The kinetic curves, demonstrating the dependence on time of the density and size of micro-crystals of Sb, as well as of the dependence on time of the size of Sb_2S_3 crystals and of fraction of the crystalline phase were obtained with the help of frame-by-frame analysis of the video. Primary crystallization of Sb_2S_3 occurs in accordance with the layer polymorphous crystallization mode with the relative length $\delta_0 \approx 4992$. The dependence on time of the fraction crystallized has a quadratic character. Secondary crystallization of



Sb_2S_3 occurs also in accordance with the layer polymorphous crystallization mode with the relative length $\delta_0 \approx 9725$. The dependence on time of the fraction crystallized can be described by power function with the exponent 0.68.

Sb_2Se_3 films under the action of electron irradiation exhibits an island polymorphous crystallization mode [2, 3] with a relative length $\delta_0 \sim 200$. Direct electron microscopic observations have shown that new nuclei appear at every step of the transformation and so-called continuous nucleation takes place (Fig. 3). Time dependence of the crystallized volume fraction has an exponential character, described by the Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation. Numerical value of the Avrami exponent nearest integer $n = 2$.

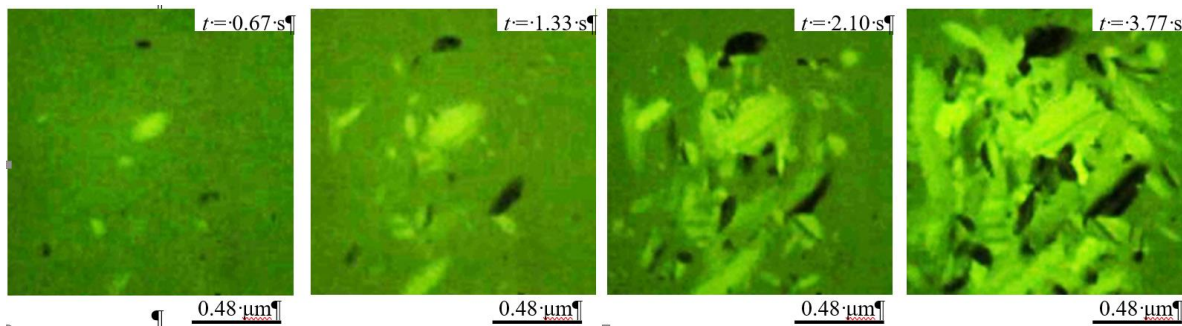


Fig. 3. Video frames of crystal growth in amorphous films of Sb_2Se_3 at electron beam irradiation. Time moments t , that has passed from the beginning of the recording of the crystallization process, are shown in the upper right corner of each frame

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I16. Energy Storage: Challenges of 21st Centuries and modification of Solid State electrolytes for next generation batteries

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All-solid-state lithium-ion batteries (ASSLB) demonstrate significant advancements in energy density and safety comparing the traditional lithium-ion batteries, which using solid state electrolyte. Smart lithium-metal batteries (LMBs) offer high capacity and low electrochemical potential, but face challenges such as imbalanced electrolyte-electrode interfaces and high risk. This study introduces a novel nanoceramic-based electrolyte fillers integrated with polyethylene oxide to form a flexible, free-standing film. This film improves battery safety and stability, showing excellent ionic conductivity, high transference number, and a wide electrochemical stability window at room temperature. The Enhanced ionic conductivity in LATP/LLTO nano fillers help build a stable solid electrolyte interphase (SEI) and prevent dendrite growth, enabling reliable performance at different current densities of without short-circuiting. The resulting battery demonstrates superior cyclic stability and high coulombic efficiency, highlighting the potential of this electrolyte design for high-performance applications.



I17. Strategies to interface an adipose-derived decellularized extracellular matrix with graphene-based materials for neural tissue engineering

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Within the framework of the European project NeuroStimSpinal, a decellularized ECM from adipose tissue (adECM) was explored to design several strategies for the challenging repair of the injured spinal cord. This talk presents two of the investigated strategies. Within the first strategy, the recreation of the nano-scaled architecture of the native tissue was targeted. adECM was first processed into nanofibers by electrospinning, yielding to bidimensional platforms, followed by gas foaming resulting in an expanded three-dimensional nanofibrous construct. Shaping adECM into a nanofibrous 3D construct was assisted by blending the adECM with lactide-caprolactone copolymers to modulate the mechanical properties towards soft, yet structurally stable, 3D constructs. In view of boosting their performance to guide neural stem cells, the nanofibrous constructs were doped with a bioinspired polydopamine-functionalized graphene oxide, which demonstrated to promote neuronal differentiation and neuritogenesis.[1] The second strategy relied on using the adECM as a biomolecular physical crosslinker to partially reduced graphene oxide to form porous constructs by a simple liquid-solid thermally induced phase separation and freeze-drying. Using partially reduced graphene oxide (rGO) enabled to control the interaction between rGO and adECM and favor neural stem cells differentiation.[2]

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I18. Synthesis and Characterization of CO₂-Stable Yttrium-Doped BaZr_{0.8-x}Sn_xY_{0.2}O_{3-δ} Proton-Conducting Electrolytes

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Barium stannates are renowned for their distinct structural and chemical properties, while also holding significant promise as proton-conducting ceramic electrolytes [1-2]. The addition of tin (Sn) offers several advantages, including improved sinterability and tolerance to carbonaceous/humidified atmospheres. This research aims to optimize the composition and structure of the system BaZr_{0.8-x}Sn_xY_{0.2}O_{3-δ} (x= 0–0.8) to clarify the impact of Sn-additions on the resultant electrochemical performance. The compositions were prepared using a solid-state route, with X-ray diffraction (XRD) analysis confirming pure phase formation across the compositional range.

The addition of Sn improved densification in air at 1600 °C, achieving ~90% densification for values of x ≥ 0.6. Electrical conductivity under nominally dry (p_{H2O} ~10⁻⁷ atm) and wet (p_{H2O} ~10⁻² atm) conditions (550 °C – 850 °C) was measured using electrochemical impedance spectroscopy (EIS), as a function of oxygen partial pressure. The partial conductivities of protons, oxygen ions, and electronic holes were determined from these results, based on a defect-chemistry model.

Samples with higher Sn content exhibited lower protonic transference numbers, consistent with their more elevated acidity and subsequent lower hydration enthalpy. This work, therefore, underscores the need to carefully balance the opposing requirements of densification and conductivity as a function of Sn-content, while also maintaining a desirable chemical stability. The transport properties of the BaZr_{0.8-x}Sn_xY_{0.2}O_{3-δ} family add significant knowledge to the field of perovskite proton conductors, allowing for a quantitative assessment of their applicability as electrolyte membranes for fuel cells, electrolyzers, and other electrochemical applications under various working environments.

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I19. Molecular dynamics simulation of graphene woven fabric/polyethylene nanocomposite

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Recently, the usage of fiber-reinforced polymer composites has been widely expanded in engineering due to their high strength and fracture toughness [1]. One of the most important reinforced polymer is graphene woven fabric/polyethylene nanocomposite (GWF/PE). But, there are many fundamental questions about physical properties of GWF/PE. Therefore, the goal of this research was to study mechanical properties as well as cohesive energy of GWF/PE using molecular dynamics simulation technique. The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package [2] used to simulate at isothermal-isobaric (NPT) ensemble at 300 K and 1 atm pressure by applying AIREBO potential. The open visualization tool (OVITO) was used to visualize the trajectories of particles [3]. The temperature of system was controlled by Nose-Hover thermostat. The stress-strain diagram for pure polyethylene, pure GWF, and GWF/PE composite obtained from our molecular dynamics simulation results. As a result of the pull-out test conducted for the study of the interfacial feature, the results confirmed that sandwiching GWF with PE polymer increases ribbon sliding resistance.

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I20. Reaching the reversible hydrogen storage target by regenerating the irreversible high capacity hydride LiBH₄

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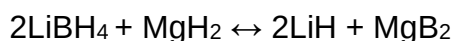
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INTRODUCTION

The green fuel, hydrogen, is an attractive replacement to hydrocarbon fuels for vehicular applications. However, unlike hydrocarbon fuels, since hydrogen occupies more space on-board storage of H₂ in light-duty vehicles is a significant challenge. The US Department of Energy (USDOE) hydrogen storage capacity target for hydrogen fuel cell electric vehicles is 6.5 wt.% H₂ (quantified with respect to the total weight of the storage tank) [1]. To achieve this capacity, various classes of solid-state metal hydrides have been explored, such as intermetallic, complex, and binary hydrides. Nevertheless, optimizing a hydrogen storage material that meets the desired target requirement has not yet been possible. Currently, the best reversible material known in the literature is MgH₂ which provides an experimentally reproducible capacity of 6 wt.% H₂ (theoretical capacity: 7.6 wt.% H₂) [2]. However, accounting for at least a 20% weight contribution from the empty tank and system components, a 6 wt.% material (hydride) capacity means a system capacity of 4.8 wt.%, which falls short of the USDOE targets for hydrogen vehicles. In this context, our current study focuses on a promising high capacity hydride system, called reactive hydride composite (RHC), 2LiBH₄ + MgH₂. This RHC releases 11.4 wt.% hydrogen as per the following reaction, which also can be reversibly stored,



However, the hydrogenation/dehydrogenation reactions show kinetic limitations which necessitate high operational temperatures and pressures (typically greater than 400 °C and 100 bar hydrogen). In the present study, we have replaced a small quantity of MgB₂ with TiB₂ and evaluated the hydrogen storage capabilities of the LiH/MgB₂/TiB₂ nanocomposite. Our detailed analyses suggests that the incorporation of TiB₂ significantly promotes the hydrogen storage characteristics of the LiBH₄/MgB₂ RHC system.

EXPERIMENTAL

The samples taken as per the required values of x for the formula unit, 2LiH + (1-x)MgB₂ + xTiB₂, where x = 0, 0.25, 0.5, 0.75 and 1 were ball milled using a planetary milling facility Retsch PM200 (rpm: 350, ball to powder ratio: 70:1, time, 5h). Hydrogen storage characteristics were tested by Sieverts volumetric technique and the structural characterization was performed by X ray diffraction facility (Rigaku). All the powder processing was performed inside an Ar filled glovebox.

RESULTS AND DISCUSSION

The reactive mixture with the formula unit 2LiH + (1-x)MgB₂ + xTiB₂ (x=0, 0.25, 0.5, 0.75, and 1) was ball milled for 5 hours. Subsequently, each sample was hydrogenated at



370°C / 70 bar H₂ for 5 hours, and the phase-structural features, before and after hydrogenation, were tested by XRD technique. The XRD analyses revealed the presence of LiBH₄ and MgH₂ within the values $x=0-0.5$. The dehydrogenation experiments by Sieverts volumetric technique reveal that the samples with $x=0.05$ and 0.15 stores 9.2 wt.% H₂. We have observed fast kinetics up to 3 wt.%, followed by a slower kinetics for the remaining quantity of hydrogen when dehydrogenation was performed at 406°C/5 bar H₂. The desorption process shows two steps in all the cases of “x” tested in the current study, which lead us to believe that the initial step might involve the independent dehydrogenation of MgH₂. Regarding the reaction kinetics in the second step, the TiB₂-added samples exhibit improved kinetics compared to the samples without TiB₂. It is also worth noting that the presence of TiB₂ in these samples enhances the abundance of restored hydride phases (LiBH₄ and MgH₂), which is proven by repeated hydrogenation experiments.

CONCLUSION

The hydrogen storage performance of the composite 2LiH+MgB₂ is improved by the addition of TiB₂. When 0.05TiB₂ is added to the composite 2LiH+0.95MgB₂, it becomes possible to store 9.2 wt.% H₂. The dehydrogenation kinetics at 406 °C with 5 bar H₂ back pressure is found to be better for 2LiH + 0.95MgB₂ + 0.05TiB₂ as compared to any other samples tested in the current study.

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I21. Composite hydrogels based on graphene oxide and biopolymer as adsorbents: applications in separation processes

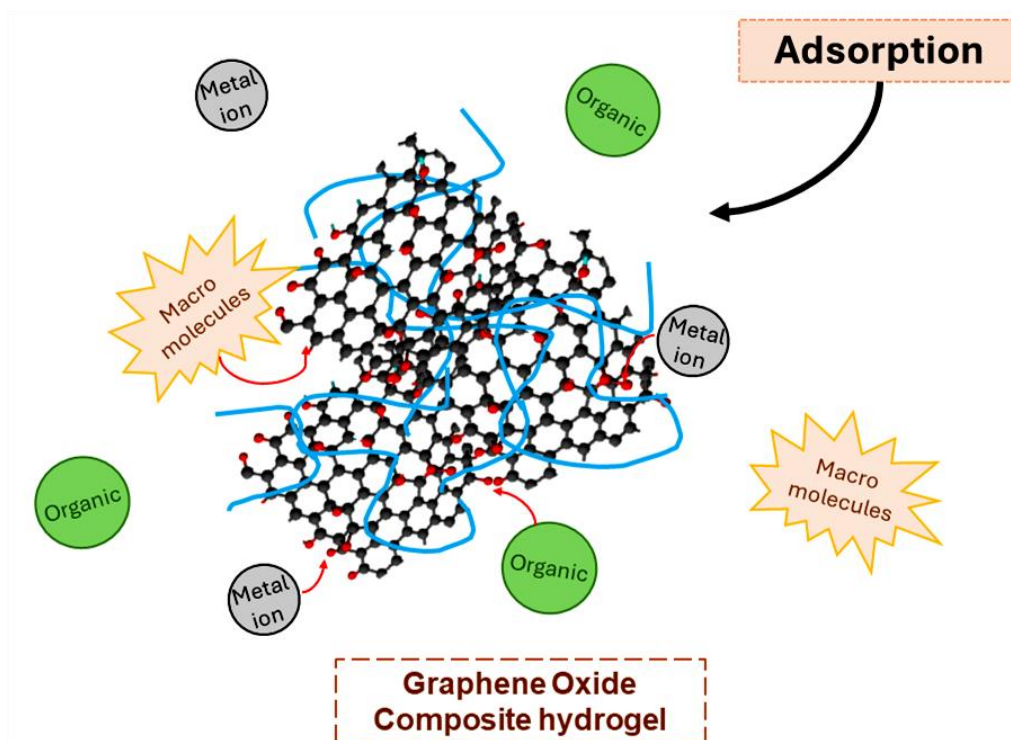
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Due to recent advances in developing technologies for carbon nanomaterials production, the viable application of these materials in continuous and industrial processes is becoming more realistic. Because of their properties, graphene-based materials have proved to be promising as adsorbents for both the simpler and more complex organic substances; as well as some inorganic compounds. Thus, this work aims to demonstrate the development, focusing on the application of composites using graphene derivative, for applications in continuous separation processes, from water treatment to protein capture. Overall, the hydrogels prepared using graphene oxide (GO) and biopolymer revealed evidence of GO interaction with the polymer that constitutes the matrix, resulting in 3D material. The hydrogel composite was tested as an adsorbent and showed promising results for the adsorption of several synthetic dyes, including methylene blue, Nile blue, safranin O; in addition to the drug chloroquine and its precursor quinoline, and heavy metal ions, such as Cd^{2+} . For dyes, the adsorption capacities achieved in a fixed bed column were greater than 79 mg.g^{-1} , going up to $\sim 225 \text{ mg.g}^{-1}$ [1,2]. Furthermore, the material also presented relevant results with regard to the capture of hemeproteins, presenting adsorptive capacity values in a fixed bed column that were higher than 385 mg.g^{-1} for cytochrome C, and 340 mg.g^{-1} for myoglobin [3]. The adsorption mechanism behind that is possibly mainly related to the electrostatic interactions between the highly negatively charged GO composite hydrogel and the positively charged adsorbates. The 3D material proved to be an interesting viable alternative to be used in continuous separation processes, whether for water treatment, or capturing substances, since most of the composite was also biodegradable and the material exhibited remarkable regenerative capacity and reusability. Moreover, a small amount of material (less than 0.5 g, on a dry basis) can be used to adsorb and capture several cationic organic dyes, some pharmaceuticals, hemeproteins, and heavy metals from water. All that proves its potential effectiveness for applications in separation processes.



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I22. Organized functional nanomaterials for energy applications

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Amidst the growing energy demand and the potential impact of its production on global warming, advancing materials for energy harvesting and efficient storage is vital for sustainable progress. While batteries and supercapacitors are commonly utilized for this objective, their energy storage capacity is restricted by their low power density. Among current energy storage devices, dielectric capacitors are attractive alternatives with a stable, ultrahigh power density of the order of 10^8 W/kg and fast charge-discharge cycles, suitable for hybrid electric vehicles, wearable electronics, medical devices etc. [1,2]. Relaxor ferroelectric (RFE) thin film devices with higher breakdown strength and electroactive polymer nanocomposites (PNCs) of PVDF-family are attractive for light weight, flexible storage. The processing of PVDF is pivotal in regulating its polymorphic forms and breakdown behavior.

This research focuses on exploring the energy conversion mechanisms through magnetoelectric coupling and analyzing the storage characteristics of RFE thin films and multiferroic PVDF PNCs.

We developed Aurivillius RFE thin films by pulsed laser deposition and PNCs by compression molding. Ferroelectric nanofillers with $\text{Ba}_{0.7}\text{Ca}_{0.3}\text{TiO}_3\text{-Co}_{0.6}\text{Zn}_{0.4}\text{Fe}_2\text{O}_4$ were introduced to realize magnetoelectric (ME) PNCs. X-ray diffraction and FTIR were used to assess crystallization of PNCs while TEM and AFM were used for dimensions and morphological studies. Energy storage and breakdown analysis was performed experimentally, and results were understood via simulations.

RFE thin films exhibited high fatigue endurance up to 10^{10} cycles and energy storage density > 95 J/cm³. Thermal stability and fatigue-free storage were also observed.

The progressive increase of nanofiller content has led to enhanced polarization (11 $\mu\text{C}/\text{cm}^2$), soft ferromagnetic properties, and enhanced ME coupling of 59 mV/cm-Oe due to switchable magnetostriction at lower saturation field of 1.2 kOe. Detailed energy storage characteristics confirm that the nanofiller inclusion up to 7.12 vol% effectively improved the recoverable energy storage density (21.2 J/cm³) with an efficiency of 67%. The experimental and simulation results corroborate a significantly improved breakdown strength of 617 kV/mm with reliable performance. Thus, careful processing provides viable polymer dielectrics with beneficial storage characteristics [2].

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123. Recyclable Photon Upconversion Crystals Doped Bacterial Cellulose Composite Films for Sustainable Photonics

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Biopolymers currently utilized in photonics are predominantly confined to linear optical color responses. This study aims to expand the potential of bioplastics in nonlinear optical applications. To demonstrate this, we opted for triplet-triplet annihilation photon upconversion (TTA-UC) as a nonlinear optical process. TTA-UC converts two low-energy photons into one high-energy photon and is utilized in photon harvesting and storage. To perform a proof-of-concept demonstration, a bacterial cellulose film (BC) was grown by culturing the bacterial strain *Komagataeibacter xylinus*. TTA-UC crystals of the chromophore (PdTPBP: DPA, sensitizer: annihilator) were cultivated on BC hydrogel, then coated with gelatin (G) and dried to improve optical transparency by adjusting the refractive indices. TTA-UC crystals enclosed within the BC-G bioplastic film show upconversion of 633 nm red light to 443 nm blue light, with a quadratic to linear dependence on excitation power density. Importantly, this pre-programmable assembly-disassembly technique facilitated the retrieval of DPA at end-of-life (EOL) through physical separation or anti-solvent bathing which was reused to complete the circular loop. The remaining clean biomass was subjected to biodegradation in the natural environment following the principles of a circular bioeconomy.



I24. Properties of Li- and Mn-doped Potassium Tantalate Polar Dielectrics

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Alkali tantalates, such as KTaO_3 (KT) and LiTaO_3 , are members of the ferroic family of lead-free compounds with potential applications for electronic components and tissue engineering, respectively [1,2]. Their solid solution, $\text{K}_{1-x}\text{Li}_x\text{TaO}_3$, wherein displacements of small Li ions on K sites generate strong local dipole moments, which couple electrostatically to the KT polar soft mode, has also been intensively studied. Therefore, both dielectric relaxations and ferroelectric phase transition were reported for heavily Li-doped KT [3-5]. Only the relaxation was, however, reported for $\text{K}_{1-x}\text{Li}_x\text{TaO}_3$ with $x < 0.008$ as well as for weakly (0.01–0.3%) Mn-doped KTaO_3 single crystals [6]. Analogically, the origin of the relaxation was shown to be the off-centre displacement of dopant ions on the K site in one of the six $\langle 001 \rangle$ -type crystal directions. In addition to the single crystal results, low-frequency dielectric relaxations were further observed for Li- or Mn-doped KT ceramics [3,7,8]. However, in contrast to $\text{K}_{0.98}\text{Li}_{0.02}\text{TaO}_3$ ceramics, no ferroelectric phase transition was detected in polycrystalline $\text{K}_{0.985}\text{Mn}_{0.015}\text{TaO}_{3\pm\delta}$ [7], while magnetoelectric effect was observed in $\text{K}_{0.97}\text{Mn}_{0.03}\text{TaO}_{3\pm\delta}$ ceramics [8]. Moreover, KT single crystals co-doped with 0.27% Li and 0.15% or 0.31% Mn determined by inductively coupled plasma spectroscopy analysis were found to present separate low-frequency dielectric relaxations of comparable strength in KTaO_3 in contrast to other co-doped KTaO_3 single crystals [9]. The relaxation dynamics follow the Arrhenius law with activation energy values of ~ 77 and 107 meV, attributing the relaxation origin to the dipoles formed by off-centre Li^+_{K} and $\text{Mn}^{2+}_{\text{K}}$ ions, respectively.

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I25. Combining Electrochemical Deposition and PVD Coatings Towards Chromium (VI) Replacement

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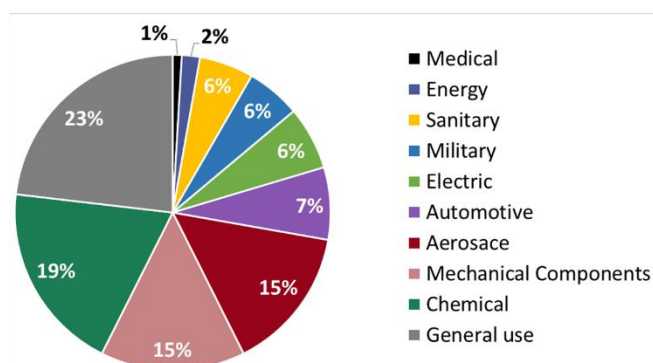
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Chromium trioxide or hexavalent chromium is a chemical compound widely used in industry. Nonetheless, it has been considered as a substance of very high concern and included in the European union REACH Regulation (EC) No 1907/2006 (annex XIV). Ultimately, a proper compound and/or technology are required to progressively replace the use of hexavalent chromium.

Electroplating using solutions containing trivalent chromium is the most explored technology to be used as an alternative to hexavalent chromium. Other technologies such as PVD, nickel electro/electroless plating, and thermal spraying are also alternative candidates.

This work briefly reviews the industrial transition from hexavalent chromium coatings towards more sustainable alternatives, including the most promising contenders to hexavalent chromium coatings. Moreover, preliminary results concerning electrochemical deposition followed by PVD coatings demonstrate the practicality of such an option within the industrial sector for decorative purposes. Nevertheless, the compulsory chromium (VI) replacement by the combination of both technologies still requires numerous improvements.



Pie chart segmentation of the granted used of hexavalent chromium per industry sector

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I26. Metallic foams as a substrate in the electrochemical technologies

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The selection of the materials for substrate is generally based on the end-application. Due to its porous structure, research on metallic foam is a popular topic due to its diverse industrial applications and unique combination of properties. There are two types of metallic foams: closed cells and open cells foams. Closed-cell foams provide good mechanical properties but do not allow access to their internal surface, whereas open porosity is generally required for functions associated with the interior of the material and are mostly used in functional applications where load-bearing capability is not the primary goal.

The important characteristic of applied foams is an electrochemically active area (EAA). It can be determined by the electrochemical impedance spectroscopy. EAA depends on the limiting stage of process occurring on the electrode. It was determined to be 7–14 times higher than that for the flat electrode, whereas charge transfer resistance on the Cu foam electrode is 1.5–1.7 times lower than that on the flat electrode: mass transfer and deposition rate is up to 3 times higher on the foam surface in comparison with a flat surface.

The applicability of Cu-foam electrodes for electrowinning of based metals from the leachate of electronic waste in citric solutions, as well as supports for electrodes used in electrocatalytic processes will be discussed.

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I27. Unveiling the impact of the size and morphology of levodopa-functionalized gold nanourchins in their in vitro cytotoxicity

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Gold nanoparticles (AuNPs) are widely recognized as one of the most extensively researched metallic nanomaterials owing to their exceptional biocompatibility. Their versatility extends to various medical applications, including drug and gene delivery, as well as photothermal therapy (PTT) [1]. Moreover, they hold promise as a novel candidate for the development of drugs targeting Parkinson's disease (PD) [2]. Levodopa, a dopamine precursor, stands as an effective and well-tolerated agent for replacing dopamine in PD treatment [3]. Notably, it can be used in the synthesis of levodopa-functionalized multi-branched gold nanostructures [4]. Hence, the pursuit of environmentally sustainable methods to produce these anisotropic gold nanostructures, ensuring precise control over size and morphology, becomes imperative. Simultaneously, verifying their safety and efficacy is essential, considering their potential utilization in the biomedical field.

In this study, we present for the first time the novel synthesis of Au nanostructures, specifically nanourchins, using levodopa extract derived from *Mucuna pruriens*. Initially, we explored the influence of various reaction parameters, such as the concentrations of gold seeds, gold salt, and levodopa extract, on the resulting AuNPs' morphology, size, and stability. Employing an experimental design approach, we identified the critical parameters necessary to achieve targeted morphologies with precise size control. Notably, we observed that a low seed concentration combined with a high levodopa concentration yielded larger nanourchin structures. In contrast, a high seed concentration paired with a low levodopa concentration resulted in spherical morphology. Subsequently, we conducted a cytotoxicity assessment of the functionalized levodopa Au nanourchins nanostructures, comparing those with higher (100 nm) and lower (40 nm) sizes with nanourchins synthesized using commercial levodopa, as well as spherical AuNPs, for comparative purposes. Our findings highlight the potential of these biobased gold nanostructures in the development of efficient and reliable drugs for treating Parkinson's disease.

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I28. The bright future of Carbon Dots for biomedical and environmental applications

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Since the discovery of carbon dots (CDs), significant research efforts have been directed towards exploring their potential in various applications. This is because of their high biocompatibility, good water solubility, low toxicity, low photobleaching, high fluorescence stability, and minimal environmental impact. Functionalization of CDs with other active molecules or ions has increased the potential applications of nanohybrids. These methods allow for precise control of the size, shape, and surface functionality of CDs, enabling fine-tuning of their properties for specific applications.

This lecture aims to highlight the impact of scientific research on the development of CD-based materials, focusing on improving their performance and/or extending their range of applications in biomedical and environmental fields. Special attention should be given to the synthetic pathways used to create new conjugates. In the biomedical field, CDs have shown great promise for applications such as targeted drug delivery, bioimaging, and photodynamic therapy. In environmental applications, CDs have demonstrated potential for pollutant detection, water purification, and environmental monitoring. Their high fluorescence stability and sensitivity make them excellent candidates for the development of sensors capable of detecting trace amounts of environmental pollutants. Several examples are provided to underscore the relevance of these nanomaterials in developing a more advanced and sustainable society.

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Oral presentations



O1. DNA identification using surface enhanced Raman scattering (SERS): different types of SERS DNA sensors

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The deoxyribonucleic acid (DNA) is the carrier of genetic information for all living organisms. Even a small mutation in DNA sentence can cause many diseases. Therefore, developing sensitive, fast and precise methods for detection of DNA mutations is very important from a practical point of view. A promising method for detection of specific DNA fragments is surface-enhanced Raman scattering (SERS) [1-4]. In SERS spectroscopy, if molecules of some analytes are located at or near the surface of nano-structured plasmonic materials, the efficiency of the generation of Raman signal can be increased by many orders of magnitude. In some cases, the efficiency of the generation of Raman signal in the SERS effect is so large, that it is possible to record a good quality Raman spectrum even of a single molecule [5]. Therefore, SERS spectroscopy is one of the most sensitive analytical tools.

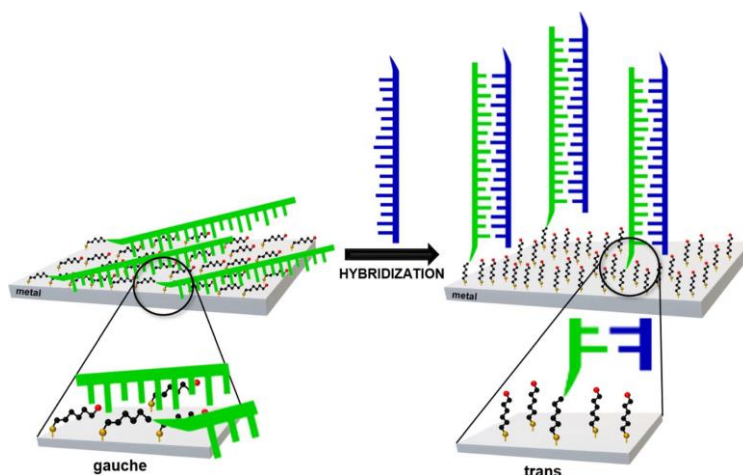


Figure 1. Scheme of the SERS DNA sensor based on rearrangement of the alkanethiol chains (alkanethiolate linking moiety of single stranded DNA and 6-mercaptohexan-1-ol). Reprinted from ref. [3]. CC BY license.

In this presentation some methods of detection of various DNA fragments using SERS spectroscopy will be described. We focus especially on developed by us methods based on hybridisation-induced rearrangement of the alkanethiol linking moieties via which capture single stranded DNA chains are attached to the surface of the plasmonic SERS substrate and the rearrangement of the chains of 6-mercaptohexan-1-ol which is also usually chemisorbed on the surface of the plasmonic metal to eliminate the direct interactions of nitrogenous bases of DNA with the metal surface. The scheme of the SERS DNA sensor utilising the rearrangement of the alkanethiol chains (alkanethiolate linking moiety of capture single stranded DNA and 6-mercaptohexan-1-ol) during DNA hybridization is shown in Figure 1. That rearrangement is indicated by a characteristic



change in the measured SERS spectrum. Developed new SERS DNA (bio)sensor has been tested on clinical samples and is characterized by the low detection limit at the level of $\mu\text{g/L}$, wide analytical range from ca. 7 $\mu\text{g/L}$ to ca. 70 mg/L and high selectivity.

Acknowledgments

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O2. The beneficial effects of CeO₂ NPs integration on the microstructure and corrosion behavior of electrodeposited nickel coatings

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Corrosion is a pervasive issue affecting various metal structures, prompting the development of protective coatings to mitigate its impact. The current research was conducted in order to improve the surface properties, hardness, wear resistance and electrochemical corrosion resistance of Nickel coatings. To this end, Ni-CeO₂ layers were electrodeposited on copper substrates by chronopotentiometry from a watts bath at a current density of 50 mA/cm². Fourier-transform infrared (FTIR) and Raman spectroscopy were employed to analyze the chemical composition and bonding structures of the Ni-CeO₂ coatings, and the X-ray diffraction (XRD) was used to examine the crystallographic structure of CeO₂ NPs. While The surface morphology of the Ni-CeO₂ coatings was assessed by optical microscopy and the surface roughness parameter Ra was determined using a Keyence VHX-7000 digital microscope. The electrochemical behavior and the corrosion properties of the deposits in 0.5N NaCl were investigated by means of d.c polarization measurements, open circuit potential and electrochemical impedance spectroscopy (EIS). It was found that the incorporation of CeO₂ NPs into the nickel coatings resulted in a significant enhancement of corrosion resistance. The EIS data demonstrated increased impedance, indicating a reduction in the corrosion rate. Tafel analysis further supported these findings by revealing lower corrosion current densities for the Ni-CeO₂ coatings compared to pure nickel.



O3. Photocatalytic degradation of methylene blue using carbon-based materials

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Water is the basis of life and regulates the ecosystem. Access to potable water is threatened by economic challenges, the world's population growth, and faster climate change on the Earth. Industries are significant water consumers and reduce their accessibility. Industrial chemical pollutants like textile dyes are released into the water environments and may harm humans and the biosphere. Their removal from water is of essential importance for the ecosystem [1].

Amongst the advanced oxidation processes (AOPs), solar-driven photocatalysis has shown interesting outcomes concerning its application in removing persistent pollutants from wastewater. TiO₂ has been widely used to promote photocatalytic reactions. However, there are some disadvantages concerning its full-scale implementation that fall mainly into high band gap energy and fast recombination rate of electrons and holes [2]. For a better contribution, photocatalysts with appreciable light harvesting properties, slow recombination of photogenerated charge carriers, and fast charge consumption during redox reactions are necessary. The need for a potential photocatalyst for large-scale and industrial use suggests carbon, as it is sustainable, economical, and environmentally friendly. Carbon has been widely used in various forms (graphene and graphitic carbon nitride) due to its excellent properties, such as physico-chemical, thermal, and electron mobility [3].

The presented study aims to investigate the removal of the industrial chemical pollutant MB, a textile dye applied worldwide and detected in water environments, which was utilised as the target pollutant in the photocatalytic process. Accordingly, under simulated Solar irradiation (300W Osram Ultra Vitalux bulb), heterogeneous photocatalysis was carried out inside a modified beaker reactor with prepared carbon-based material photocatalysts in the form of suspension and film. The results of performed tests show the efficient removal rate (more than 90%) of MB dye using different prepared carbon-based catalysts in both forms. Using powders as photocatalysts raises challenges related to their full recovery for reuse and limiting their application in the environment. Although immobilised films have a smaller specific surface area than powders, they are easier to regenerate and reuse with a similar removal efficiency. Underlying this research was also a success of the full-scale viability of solar photocatalysis for its practical applications in wastewater treatment using carbon-based materials.

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O4. Perovskite Anodes for Biogas-Powered SOFCs: CaVO_3 , SrVO_3 , SrMoO_3

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Rare-earth and alkaline-earth vanadates and molybdates with perovskite-like structures attract attention for their potential application as redox-reversible components in fuel electrodes of solid oxide fuel cells (SOFCs) [1-2]. Components derived from $(\text{Ln},\text{A})\text{VO}_y$ (where A is an alkaline-earth metal cation) are particularly interesting for natural gas- and biogas-fueled SOFCs due to their anticipated resistance to deactivation by carbon deposition and sulfur-containing impurities. This study aims to comparatively assess a series of perovskite-type compounds— $\text{SrVO}_{3-\delta}$, $\text{SrMoO}_{3-\delta}$, and $\text{CaVO}_{3-\delta}$ —as potential anode components.

The ceramic materials were synthesised via a solid-state reaction route under controlled atmospheres. Particular attention was given to the synthetic procedure to ensure the preparation of phase-pure perovskites. The ceramic samples for characterization underwent sintering between 1350°C and 1500°C under reducing conditions. The crystal structure and microstructure of the prepared materials were characterized using X-ray diffraction (XRD) and scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM/EDS). Furthermore, thermomechanical compatibility with solid electrolytes was assessed through controlled-atmosphere dilatometry. Electrical conductivity was assessed as a function of temperature and oxygen partial pressure within the phase stability domain of the perovskite phase. Additionally, high oxygen partial pressure ($p\text{O}_2$) stability boundaries at operationally relevant temperatures were determined during the electrical measurements. The redox behavior during cycling between reducing and oxidizing atmospheres was evaluated through conductivity relaxation, thermogravimetry, and dilatometric studies, complemented by room-temperature X-ray diffraction (XRD) and microstructural inspection. The properties of the materials are analyzed for their suitability for application in solid oxide fuel cell (SOFC) anodes.

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O5. Structural variety of metals as a cause of the variety of oxidation states and coordination number: structural analysis of selected ruthenium complexes

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In contrast to the quantum mechanical model which describes through the s, p, d, f orbitals the probable position of a single electron, the presented model, based on crystallographic data, describes the probable optimal symmetry of the placement of a group of electrons for achieve the structural stability of the atom, to better adapt it to different physical/chemical conditions. This mechanism determines the elasticity in the management of the position of the electrons and consequently in the structure of the atomic building almost nothing is fixed.

However, the following basic structural mechanisms by which atomic shells are formed can be identified:

- shells which have the role of forming a supporting structure built by localized electrons through the symmetrical placement of the electrons in the bilobed orbitals and around the nucleus (shells called θ , theta); based on the quantity of electrons that perform this role and regardless of the block they are distributed with the following symmetries (to make the representation of the "supporting" structures that form the electrons more effective, an electron will be drawn as a cube):

Tab. 1. The most frequent symmetries of θ shells.

simple θ shells	cube = 8 electrons 	octahedron = 6 electrons 	cubooctahedron = 12 electrons 
composite θ shells	octahedron + cube = 14 electrons 	octahedron + cubooctahedron = 18 electrons 	

- shells that perform the role of division and protection of the θ shells, built by mobile electrons with spherical orbitals (shells called τ , tau). In addition to the s-block electrons, this type of shell often also are formed from the first two electrons of the d-shells and f-shells (nd1-2, nf1-2).

Coordination compounds are formed to complete the outer shells of coordinating atoms by sharing a single electron between two orbitals of two atoms forming the coordination bond.

With the introduction of these theoretical postulates, an interpretation of the causes of the following properties of coordination compounds is proposed, with the examples of selected ruthenium complexes: structural variety, variety of oxidation states of coordinating atoms, variety of coordination numbers, pseudo-hyper-valence of shells, as illustrated in table number 2.



Tab. 2. The most frequent symmetries of ruthenium θ shells in selected complexes (Composition of composite shells has illustrative value), oxidation states of ruthenium and coordination numbers.

RuO_4	RuCl_6	$[\text{Ru}(\text{H}_2\text{O})_6]^{2+}$	H_2RuO_4 $[\text{RuCl}_8]^{2-}$	$[\text{RuCl}_6]^{2-}$ $[\text{RuO}_3]^{2-}$	$\text{Ru}(\text{CO})_5$
internal spherical shell τ					
$4s_{1-2}$	$4s_{1-2}$	$4s_{1-2}$	$5d_{1-2}$	$5d_{1-2}$	absent
composition of the external θ shell					
$4p_{1-6}$ $4d_{1-6} + 5s_{1-2}$	$4p_{1-6} + 4d_{1-2}$ $4d_{3-6} + 5s_{1-2}$	$4p_{1-6} + 4d_{1-6}$ +6 electrons	$4d_{3-6} + 5s_{1-2}$ +2 electrons	$4d_{5-6} + 5s_{1-2}$ +2 electrons	$4d_{1-6} + 5s_{1-2}$ +4 electrons +6 electrons
oxidation states of ruthenium					
VIII	VI	+2	VI	IV	-10
coordination number					
4	6	6	4, 8	6, 3	5

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O6. Rheological Properties of Cement Pastes Mixtures with Mixed Oxide Additives

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Cement-based products are the most widely used synthetic materials by humans, and the production of cement clinker is a process of high-energy consumption and significant emission of greenhouse gases¹. The main challenge in this sector has been the mitigation of harmful environmental effects, leading to intensified searches for eco-efficient materials. Layered double hydroxides (LDH) are synthetic (nanostructured) clays that have shown able to improve some properties of cement pastes and composites¹. This study demonstrates the effectiveness of incorporating mixed oxides (MO) derived from LDH in optimizing the rheology of cement pastes. Thermal aging of LDH allowed the preparation of MO with different specific surface areas (SSA) that were incorporated into Portland cement at different quantities. Results showed the low proportion of MO with low SSA the additive increased the paste workability by 22%. In contrast, high proportions of MO with high SSA led to a 2.4-fold acceleration in cement consolidation. The matrix-additive interactions, with the memory effect of LDH, play important roles in the hydration process of cement and the competition for the absorption of free water in the cement paste. MO materials have proven to be easily adaptable and are promising additives in manufacturing to obtain eco-efficient materials.

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O7. Enhancing MICP Self-Healing Concrete by Optimizing Carbonate Precipitation

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Due to the widely discussed problem of concrete crack formation, an intensively developing field of science is self-repairing cement composites [1]. Microbial carbonate precipitation is considered one of the sustainable methods for repairing concrete [2]. The main objective of the study was to investigate the possibility of improving the MICP process by optimizing process conditions, specifically by selecting the concentration of reaction precursors (urea, calcium lactate, and calcium and magnesium nitrates). The effectiveness of carbonate precipitation was studied using spores of an environmental bacterial strain (*B. subtilis*) under conditions without a cement composite and directly on cracked cement mortar beams. In the first stage, the precipitation rate was studied in a solution with unmodified pH and in a solution with pH = 11. A solution without the addition of bacteria was used as a control test. The mass of precipitates, along with the analysis of mineralogical composition and microstructure, were used as criteria for evaluating the effectiveness of the processes. In the second stage, cement mortar beams containing bacterial spores added to the matrix on bacterial carriers were immersed in reaction precursor solutions, and the processes taking place were cyclically evaluated (between 0 and 28 days after immersion) based on the degree of sediment filling the cracks (using ImageJ software). Weight measurements of precipitates indicated that including bacterial spores in each solution positively influenced both the quantity and quality of precipitates. The formation of mainly calcite, vaterite, aragonite, and brucite was observed. Additionally, the research demonstrated that utilizing the *B. subtilis* strain along with specific nutrients resulted in over 90% crack sealing, affirming the effectiveness of microbial repair for cement mortar cracks.

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O8. Composite materials synthesis for dye adsorption: Optimization by Box-Behnken experimental design and implications for water treatment

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Research on composite materials for dye adsorption holds promising prospects for water treatment. This abstract focuses on optimizing the synthesis of these composite materials using a Box-Behnken experimental design, a statistical method efficient for simultaneously evaluating multiple variables. The characteristics of composite materials, such as their morphology, specific surface area, and composition, are analyzed to determine their dye adsorption efficiency.

The results demonstrate that optimized composite materials exhibit maximum dye adsorption capacity, thereby offering potential solutions for treating contaminated waters. This approach carries significant implications for the development of more efficient and environmentally friendly water treatment technologies.

Adsorption removal is one of today's most important separation technologies. This study concentrated on the adsorption of a basic dye onto a composite material to determine optimal points for several physico-chemical parameters. The study of the influence of physico-chemical parameters (contact time, initial dye concentration in solution, pH, adsorbent mass, temperature) on dye adsorption capacity on the composite material showed that dye adsorption equilibrium time is achieved in less than 30 minutes and that adsorption capacity increases with increasing initial dye concentration. To establish the best-fitting isotherm, experimental equilibrium data were analyzed using several multi-parameter isotherm models. The models used include Langmuir, Freundlich, Temkin, and Elovich. Results indicate that the Langmuir model has a better correlation coefficient. Kinetic adsorption data were also examined using various kinetic models. The pseudo-second-order model was found to be the best for predicting experimental data. Thermodynamic study shows that adsorption is exothermic. To reduce the number and cost of tests, a parametric optimization of dye adsorption on the composite material was carried out using a complete factorial design with two levels. Overall, these results demonstrate the interesting dye adsorption capacity of the composite material. This can play a significant role in the depollution of colored effluents.



O9. Investigation of Damping in Porous Metal Foams

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Damping in materials and structure is known by the dissipation of energy over time under eventual action of an excitation called force. It is crucial characteristics in various engineering applications including civil engineering, mechanical engineering and aerospace engineering. It contributes to the safety, performances and longevity of these structures as well as the designed damping systems can improve the comfort and reliability of a wide range of engineering applications from everyday vehicles and machine to large scale engineering projects. The aim of this work is to investigate damping mechanism in porous metal foams, the influence of different parameter such as porosity and microstructure on the damping phenomena and some practical implications. This research unlocks full potential of metal foams for vibration control and energy dissipation, advancing engineering solutions for a wide range of industries.



O10. The Sulfuric Acid Etching Effect of Fly Ash/SiO₂ as Anode for Li-ion Batteries

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- Abstract

In this study, fly ash/SiO₂ composites were produced by simple co-precipitation without annealing process. Sulfuric acid etching of fly ash powders was applied to investigate its effect on the fly ash/SiO₂ anode performance in Li-ion batteries. Structural, morphological and electrochemical properties of fly ash/SiO₂ nanocomposites were investigated by XRD, SEM and battery tests were realized in half-cell configuration.

- Introduction

In the last 10 years, with the increasing preference for alternative energy sources and electric vehicles, the rapidly increasing demand for energy storage systems has also been noticeable. The rechargeable batteries included in these systems (Li-ion batteries, Na-ion batteries, Li-S batteries, etc.) it offers activities in a wide range of fields from the electric hybrid vehicle sector to wind turbines. Li-ion batteries (LIBs) have dominated the energy market for decades with increasing new type electrode designs. However, the complex preparation process and the serious volume expansion (~400%) of existing Si-based anode materials causes problems about sustainability considerations when designing future electrode materials [1]. Moreover, the formation of lithium dendrites and the serious safety risks-poor performance of conventional graphite anode (372 mAh g⁻¹) limit its development in practical applications [2].

On the other hand, one of the most important environmental problem (greenhouse effect, climate change, etc.) is the recycling of toxic and waste materials at the present time. Among them, coal volatile gases released by thermal reactors in particular (despite filtration systems) pose a serious danger (environmental, public health) for the regions where they are located.

The subject of this research is to introduce fly ash /SiO₂ nanocomposites to the energy sector, which will be obtained from coal fly ash taken from thermal power plants of the Canakkale region. In order to investigate the anode performance in Li-ion batteries, the etching of the fly ash effect with sulfuric acid was performed. The possible contribution of fly ash/SiO₂ nanocomposites were determined to green energy technology within the scope of the study.



- Method

There are two production stages, one is sulfuric acid etching of fly ash and another is fly ash/SiO₂ nanocomposites synthesis with co-precipitation. In this experiment, fly ash was modified with H₂SO₄ (1.0 mol/L). These samples were labeled as PFA (pure fly ash) and SFA (Sulfuric Acid Modified Fly Ash). Weight ratio of fly ash/ SiO₂ is [2/0.21]. Simple co-precipitation technique was applied to obtain fly ash/SiO₂ nanocomposites.

Powder XRD measurement of samples was performed using a Rigaku SmartLab diffractometer with CuK α (1.5406 Å) radiation operating at 40 mA and 45 kV within the range of 2 θ =10°–80°. JEOL JSM-7100F-SEM was used to investigate surface morphology of the samples. The electrochemical properties was examined by using coin cell. The active material, carbon black, and polyvinylidene fluoride were mixed in proper ratio. Charge-discharge analysis of the electrodes were tested with a voltage window using a battery test system.

Results and Discussion

Rapidly developing technology brings with many pollutant problems. Among them, toxic waste management is one of the most important issues of green energy technology. A large number of thermal power plants located in Canakkale/Turkey region are unable to evaluate coal fly ash and aim to reduce emissions only with filtration systems. This study plans to design coal fly ashes as a nanotechnology material (fly ash/SiO₂) and convert them into a technologically valuable product as anode material in Li-ion batteries. The growing of SiO₂ has been observed in fly ash carriers.

Wang et.al. [3] reported that sulfuric acid activation makes fly ash have stronger adsorption capacity for escaping ammonia, and SFA maintains good specific resistance characteristics, which has good application prospects in electrostatic precipitation and air pollution control.

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O11. Optimizing Mechanical Heart Valve Efficiency: A Systematic Approach

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Mechanical heart valves are critical for treating heart valve disease, offering essential support to patients needing valve replacement. Bioprosthetic valves have a lower thrombosis rate compared to mechanical valves, leading to unnecessary lifetime anticoagulation in patients. In the aftermath of surgery, structural heart valve degeneration (SVD) of the implanted valve may become apparent, with a typical onset between 10 and 15 years post-procedure. This poses a significant concern, especially for young, low-risk individuals with a considerable life expectancy ahead [1]. Additionally, current mechanical valve designs are constrained by limitations such as structural failure, risk of thrombosis and compromised hemodynamic performance. Mechanical and bioprosthetic valves have been used clinically to date, often causing discomfort and complications related to anticoagulant uptake, immune-induced calcification and degradation [2]. Hence, innovative strategies are imperative to surmount these obstacles and enhance the durability and performance of mechanical heart valves. This study will examine the flow characteristics within heart valves and vessels through the use of the finite element method. Moreover, the research addresses the limitations of current mechanical heart valve designs, such as structural failure and thrombosis risk, and aims to improve longevity and functionality. By optimizing performance through simulations under various parameters, the study aims to create a more efficient, reliable, and patient-friendly mechanical heart valve. This study will explore prevalent concerns related to mechanical valves, such as structural deterioration and long-term complications, juxtaposed with the merits and drawbacks compared to bioprosthetic valves. The selection of materials, determination of structural properties, and optimization of functionality will be key aspects of the design process. Through simulation analysis of the valve's biomechanical performance and effects on blood flow, necessary improvements will be identified and implemented to enhance its overall efficacy. This research contributes to the development of innovative approaches for future mechanical heart valve designs, addressing the critical needs of patients requiring valve replacement surgery.



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O12. Synthesis of chitosan-PVA hydrogel as a drug delivery system and in vitro loading and release studies of resveratrol

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Abstract

In this study, chitosan (CS)-poly (vinyl alcohol) (PVA) hydrogels were prepared by the freeze-thaw method without using cross-linkers. Properties of such hydrogels like swelling capacity, flexibility, porosity, and drug loading and release capacities are affected by freezing circumstances and the polymer's types and ratios. This procedure outlines the preparation of hydrogels using a 50/50% w/w composition of CS and PVA with changes in freezing temperature (-4°C) and freeze-thaw cycles (5 freezing cycles). The hydrogels were characterized using FTIR spectra, and their swelling property and resveratrol (RES) loading and release capacities were evaluated. The results show that lowering the temperature leads to a decrease in pore size and an increase in porosity. It was found that the swelling percentage increased as the freezing temperature decreased. RES release from hydrogels was investigated and drug release was observed to continue for 72 hours.

Introduction

Hydrogels have become a focal point in the biomedical realm due to their three-dimensional network structure, high water content, soft and flexible nature, and ability to mimic natural tissues effectively. (Enoch et al., 2023)

Their resistance to dissolution in aqueous media at physiological conditions coupled with significant swelling capacity makes them versatile for various applications. Hydrogels are found in utility in wound dressings, contact lenses, hygiene products, tissue engineering scaffolds, and drug delivery systems. Depending on the intended use, these gels can be crafted from synthetic or natural polymers, or their composites to optimize their properties. The physical attributes of hydrogels, such as structure and morphology, are influenced by factors like porosity, pore distribution and pore size. On a molecular level, the type and hydrophilic group content of polymer, cross-linking density and crosslinking point type plays crucial roles in determining swelling capacity and mechanical properties. (Figueroa-Pizano et al., 2019)



Chitosan (CS) is biodegradable and biocompatible, displaying antimicrobial activity. While easily processed, its mechanical properties may be insufficient, necessitating the addition of other materials for enhanced characteristics. (Figueroa-Pizano et al., 2019)

Poly (vinyl alcohol) (PVA) is a synthetic polymer with excellent mechanical properties and biocompatibility. It can form hydrogels without crosslinking agents through the freeze-thawing method, utilizing hydrogen bonds between its -OH groups during freezing to create crystalline zones. (Figueroa-Pizano et al., 2019)

Resveratrol (RES) offers numerous health benefits, including anti-inflammatory, anti-obesity, protection against atherosclerosis, and inhibition of platelet aggregation. (Wang et al., 2024)

This innovative approach aims to enhance solubility and facilitate sustained drug release. (Issarachot et al., 2023)

Method

Initially, to prepare a 2% (w/w) CS solution was dissolved 100 mg of CS in 5 mL of 0.1 M CH_3COOH solution with continuous magnetically stirring at room temperature overnight. Simultaneously, 500 mg of PVA was solved in 5 mL of distilled water by stirring at 80 °C for 10 h. The resulting solutions were combined at a 1:1 ratio mixing until obtained homogeneous solution at room temperature. A 7 mg/mL RES solution in ethanol was then added to the hydrogel. The mixtures were poured into Petri dishes and allowed to degas at room conditions for 2 h. The hydrogels were subjected to five cycles of freezing and thawing at -4 °C. Finally, the hydrogels were freeze-dried at -46 °C for 24 h for drug release study and further characterization.

Results

In summary, CS/PVA hydrogels were synthesized without chemical cross-linking, as cross-linkers are not biocompatible and have toxicity.

The prepared CS/PVA hydrogel characterized by FTIR spectroscopy for its functional groups. According to the FTIR results of the characterization studies, all synthesis steps were completed successfully and the hydrogel swelling tests were successful. According to *in vitro* drug release tests performed for the hydrogel, drug release of RES was successfully achieved.

Discussion

The synthesis of CS-PVA-RES has imparted desired properties for drug delivery applications. The binding of RES onto the hydrogel's surface has enhanced the stability and dispersibility of the hydrogels. The loading and releasing of RES exhibited sustained release behavior, signifying the potential of this hydrogel for controlled drug delivery systems.



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O14. Hybrid Polyvinyl Alcohol-Silica Antibacterial Nanofiber Fabricated by Combined Sol-Gel and Electrospinning Techniques

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Organic-inorganic hybrids are important in many fields because they combine the desirable properties of inorganic and organic phases. In this work, Polymer-silica hybrids Nano fiber with excellent antibacterial properties were synthesized using silica and polyvinyl alcohol (PVA) through a combination of sol-gel and electrospinning methods. The nanofibers, incorporating chloropropyltriethoxysilane (CPTS), PVA, and benzalkonium chloride as an antibacterial agent, were analyzed for their morphology, chemical composition, mechanical, thermal properties, and antibacterial activity. Results indicate that factors like polymer concentration significantly influence the fibers' formation and properties. Nanofiber prepared with 8% PVA solution, showed optimal characteristics in terms of fibrous structure, mechanical strength, and antibacterial efficiency. This study highlights the potential of electrospinning in developing advanced hybrid nanofibers with diverse applications.



O16. Nano-Calcium Oxide (n-CaO) from Various Waste Bones and Cooking Oils in the Production of Biodiesel: Catalytic Performance

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Utilizing calcium oxide produced by burning and analyzing three different animal bones, the trans-esterification processes of refined waste groundnut oil (WGO) and sunflower oil (WSO) were improved. The bone samples were broken down into tiny powders with 49 nm particle sizes and then calcined at 600 °C. Calcined fish bone (CFB), calcined cow bone (CCB), and calcined chicken bone (CCHB) have all been studied using the transmission electron microscope (TEM), scanning electron microscopy (SEM), X-ray diffraction (XRD), X-ray fluorescence (XRF), Brunnar Emmet Teller (BET), and Fourier Transform Infrared Spectroscopy (FTIR) Techniques. Powdered calcium oxide (CaO) was obtained from discarded animal bones (FAMES) and used to manufacture methyl ester. Research and evaluation were done on the impact of the catalyst dose ratio on the physicochemical characteristics of the biodiesel generated, including yield, specific gravity, density, kinematic viscosity, and acid values. Sunflower-based biodiesel (SFB) with CCB 4.0 wt.% yielded 95.0%, according to an analysis of the data using the Statistical Package for Social Sciences (SPSS) software. Groundnut-based biodiesel (GNB) with CCB at 3.0 wt.% yielded 95.0%. The best optimal trans-esterification reaction conditions were a 1:6 molar oil-to-methanol ratio, a reaction time of 1 hour, a reaction temperature of 333 K, a stirring rate of 1000 rpm, and a catalyst loading of 3–4 weight percent CaO. Waste cooking oil and the calcium oxide it produces are good sources of materials that can enhance biodiesel, and comply with American standards for testing materials (ASTM).



O18. Towards Piezoelectric Oriented Fibrous Platforms for CTE: Establishing Principles for EHD Jet Printing

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The exploitation of naturally occurring phenomenon of the body holds great promise for the development of novel constructs for its support and regeneration. Amongst these, the integration of piezoelectric actuation as regulator for the electro-mechanical cardiac tissue holds significant promise for its regeneration and further development.[1], [2] Nonetheless, bridging piezoelectric actuation with tissue engineering still finds major manufacturing restrictions. Traditional piezoelectric fibrous platforms, typically produced through electrospinning, result in bundles of 2D randomly oriented nonwoven fiber mats.[3] While this technique offers scalability, it lacks precise 3D control. As such, new high precision microprinting techniques show promise with design controllability, scalability, and compatibility with diverse materials, including piezoelectric ones.

Herein, we investigated the application of electrohydrodynamic (EHD) jet printing for the fabrication of diverse 3D structures with exceptional precision and resolution (fiber diameter <10 µm) using poly-L-lactic acid (PLLA). EHD or 3D jet writing has emerged as a noncontact alternative utilizing an electric field to eject ink from a conductive nozzle onto a substrate.[4], [5], [6] Unlike melt-electrowriting, EHD printing does not rely on polymer fusion, instead, it leverages polymer solution optimization allowing for the use of a wider variety of material choices.[7], [8] To produce PLLA microfibers (1) intrinsic properties related to ink formulation and (2) extrinsic ones related to operating parameters were optimized. The solvent was chosen taken into consideration that its suitability depends on numerous factors: i) it should dissolve PLLA with a reasonable viscosity, ii) exhibit an evaporation rate facilitating fiber solidification without clogging the printing needle, iii) conduct the applied electric field. In addition, polymer molecular weight and thus surface tension were found determinant to achieve stable fiber deposition. External parameters like voltage, needle-to-substrate distance, flow rate and collecting speeds were also critical to control fiber deposition, reduce charge-charge repulsion and restorative viscoelastic forces. Neglecting to optimize these properties carefully can result in different jetting regimes occurring within a single architectural drawing. These may include fiber coiling, near-field electrospinning fiber deposition, or complex EHD jetting being observed particularly when high voltages and feed rates are employed. Nonetheless, stable PLLA microfiber deposition was attainable being possible to manufacture various 3D architectures.



Furthermore, EHD was also explored to manufacture composite microfibers by developing inks based on piezoelectric PLLA and diverse nanofillers. With this study we established manufacturing principles for EHD jet printing, opening the exploration for multiple polymers and composites to be used to produce single microfibers layered into precise 3D architectures.

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O19. Multiphasic delivery nanosystems for delivery of Li-doped albumin nanoparticles for neutron capture therapy

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Neutron capture therapy (NCT) consists of the combined action of stable isotopes (usually ^{10}B) that can be accumulated in cancer cells and a beam of low-energy neutrons that is captured by the isotope, releasing short-range radiation for an effective cancer cell rate [7]. ^{10}B isotopes have shown great efficacy as active agents for NCT, however, the low target efficiency below threshold concentration limits their pharmacological implementation [4,7]. As an alternative, some of the latest developments in this field have considered the use of lithium [2,8]. However, traditional isotope-containing drugs lack the biocompatibility and circulation time necessary for medical applications. Carbon dots (CDs) have shown biocompatibility and optical properties which are useful for bioimaging, having been used as carriers for NCT [1,5], but still present a low circulation time since their ultrasmall size (<10 nm) make them particularly susceptible to renal clearance [3]. A microfluidic approach could allow the synthesis of size-controlled core-shell nanocapsules capable of protecting CDs while keeping the particle size below 200 nm, the maximum threshold for crossing the blood-brain barrier (BBB) [6,9]. This work aimed to develop ^6Li -containing carriers encapsulated by albumin core-shell nanoparticles (CSNPs) via microfluidic synthesis. Monodisperse biopolymeric nanoparticles (NPs) were fabricated through a double co-flow microfluidic system, in which an aqueous bovine serum albumin (BSA) solution was pumped as a disperse phase against a continuous ethanol flow. A parallel glutaraldehyde solution was added before the mixture was collected and heated at 95°C for a double chemical-thermal crosslinking process. UV-Vis spectroscopy confirmed the presence of CDs, with characteristic absorption peaks around 200 and 300 nm. SEM and DLS analysis confirmed the formation of stable monodisperse NPs with a size distribution in the 100-200 nm range. The synthesized nanoparticles were fully characterized in terms of chemical composition and structure.

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O20. Biocompatible biomimetics made by the molecular imprinting of silk fibroin

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Abstract: tailor-made biomimetics, called bioMIPs, made by innovative use of the molecular imprinting technique on silk fibroin are reported. The bioMIPs were biocompatible molecular nanotraps intended for biomedical applications.

A mean to convey tailor-made molecular recognition is molecularly imprinting (MIPs) technology, that is a strategy to entail molecular recognition to a nanomaterial by means of a template-assisted synthesis [1], herein MIP technique was attempted for the first time on methacrylated silk fibroin polypeptides, used as macromolecular building blocks. A rational approach with surface response method was used to define the conditions for the synthesis of bioMIPs. BioMIPs were of nanometric size and showed high affinity (nM) and selectivity for both a small target peptide and large proteins [2,3]. Enzymatic degradation and biocompatibility were confirmed. BioMIP's synthesis proved as a general route for entailing recognition with the advantage of greener and biocompatible nanotraps. Applications in sequestering molecular players, thus counteracting effects of diseases are expected.

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O27. Development of Lyophilized Hydrogel/Nanofiber Composite Scaffold for Soft Tissue Engineering

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Abstract

In the study, polyvinylpyrrolidone (PVP) electrospun mats were added layer by layer in polyvinyl alcohol/carboxymethyl cellulose (PVA/CMC-TA) hydrogel cross-linked with tannic acid, and lyophilized. Contact angle, FTIR, XRD and SEM analyses of the produced composite scaffold were performed.

Introduction

Tissue losses occur as a result of various accidents, injuries and surgical operations. Due to the lack of tissue and organ donations, scaffolds that support the tissue regeneration process have attracted increasing attention in recent years¹. With this increasing interest, tissue scaffolds; have formed a multidisciplinary field of study that spans the fields of materials science, biomedical and medicine. Polymeric tissue scaffolds are divided into two: synthetic and natural polymeric scaffolds and the scaffolds can be produced by many methods. These are various 3D printing methods (especially injection molding and bioprinting), freeze drying, particle leaching, electrospinning, and gas foaming techniques².

Hydrogels are three-dimensional polymeric network structures and allow cells to proliferate and grow and soft tissues to develop within this polymeric network structure^{3,4}. Likewise, electrospun mats⁵ allow cells to adhere and serve as a natural extracellular matrix (ECM). The scaffolds were prepared within polyvinylpyrrolidone (PVP) nanofiber was added to the polyvinyl alcohol/carboxymethyl cellulose (PVA/CMC-TA) hydrogel solution cross-linked with tannic acid and lyophilized.

In brief, in this study; synthetic polymeric lyophilized scaffolds are aimed to help tissue regeneration by acting as ECM.

Materials Method

10%wt. PVA, and 1.6%wt. CMC was mixed in distilled water in different beakers until a transparent solution was obtained. Then, the polymer solutions were mixed and after a while, 0.5% of the total polymer, tannic acid (TA), a non-toxic crosslinker, was added.



12%wt. PVP was dissolved in ethanol under room conditions for 1 night. PVP polymer solution was filled into the syringe and 16 kV power was applied. The distance between the needle tip of the syringe and the collector was 15 cm and the feeding rate was 2 mL/h. For each layer, 0.3 ± 0.1 mL of PVA/CMC-TA hydrogel and 1cmx1cm PVP nanofiber mats were poured into the well plate. The composite was frozen at -58°C for 48 hours and then lyophilized.

Results

The inner surface of the scaffold is rough and hydrophilic (The contact angle is below 90°). In this way, a suitable environment is provided for cells to adhere and proliferate. FTIR analysis was performed to explain the chemical structure of the scaffold (Fig. 1.)

The broad peaks between $3200\text{--}3600\text{ cm}^{-1}$ correspond to N-H and O-H stretching. Another band is at 2900 cm^{-1} and corresponds to the asymmetric and symmetric valence vibrations of CH_2 . The scaffold exhibited a peak at 1604 cm^{-1} , confirming the amide I ($\text{C}=\text{O}$) expansion vibration. The C-H₂ bending vibration peaks of PVP are shown at 1426 cm^{-1} and 1289 cm^{-1} , the peaks are slightly shifted in the scaffold (1289 cm^{-1} to 1331 cm^{-1}). The (C-O)-C-OH band around 1048 cm^{-1} is marked in the spectra. In summary, the IR spectrum shows that the PVP electrospun mat was successfully added to the scaffold.

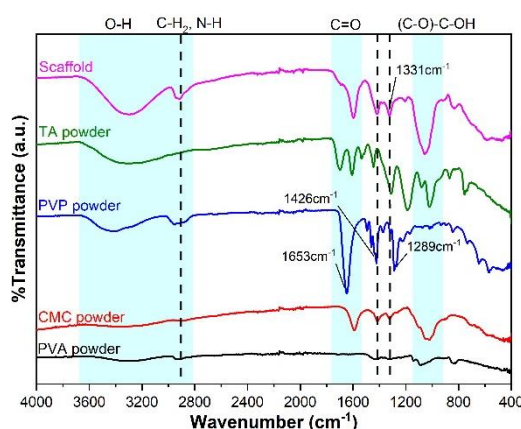


Figure 1. IR spectra of synthetic polymeric lyophilized scaffold and the scaffold components.

Discussion

Composite scaffolds prepared using the lyophilization technique exhibit ECM-like properties with the combination of excellent porosity and roughness properties of both hydrogels and electrospun mats.

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O28. Surface enhanced infrared absorption for detection of ultra-trace of 3,4-methylene dioxy- methamphetamine (MDMA)

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Abstract: Optical properties of molecules exhibit dramatic changes when adsorbed close to nano- structure metallic surfaces such as gold, silver nanomaterial. This phenomena opened a wide range of research to improve conventional spectroscopies efficiency. A well-known technique that has an intensive focus of study is surface enhanced Raman spectroscopy – SERS, as since the first observation of SERS phenomena, researchers have published great number of articles about the potential mechanisms behind this effect as well as developing materials to maximize the enhancement. Infrared and Raman spectroscopy are a complementary techniques, thus, surface enhanced infrared absorption (SEIRA) also shows noticeable enhancement of molecules in the mid-IR excitation on nonmetallic structure substrates. In their SEIRA, vibrational modes that gave change in dipole moments perpendicular to the nano-metalic substrate enhanced 200 times greater than free molecule's modes . SEIRA spectroscopy is a promising for characterization and identification of adsorbed molecules on metallic surfaces especially at trace levels. The IR reflection- absorption spectroscopy (IRAS) is a well-known technique for measuring IR spectra of adsorbed molecules on metallic surface. However, SEIRA spectroscopy sensitivity is up to 50 times higher than IRAS. SEIRA enhancement has been observed for a wide range of molecules adsorbed on metallic substrates such as Au, Ag, Pd, Pt, Al, Ni but Au and Ag substrates exhibited the highest enhancement among the other mentioned substrates.

In this work, trace levels of 3,4-methylenedioxymethamphetamine (MDMA) have been detected using gold nanoparticles (AuNPs) substrates with surface enhanced infrared absorption (SEIRA). AuNPs was first prepared and washed then mixed with different concentrations of MDMA samples. The process of fabricating the substrate prior SEIRA measurements was including mixing of AuNPs and MDMA samples followed by vigorous stirring. The stirring step is particularly crucial, as stirring allow molecules to be robustly adsorbed on AuNPs. Thus, remarkable SEIRA was observed for MDMA samples even at trace levels, showing the rigidity of our approach of preparing SEIRA substrates.

Keywords: Surface-enhanced Infrared Absorption (SEIRA) , Gold nanoparticles (AuNPs) , amphetamines, Methylene Dioxy- Methamphetamine (MDMA), Enhancement factor.

Context: The optical properties of molecules change when they are adsorbed close to metallic surfaces such as gold or silver nanomaterials. This phenomenon has led to extensive research on improving conventional spectroscopies. Surface enhanced Raman spectroscopy (SERS) and surface enhanced infrared absorption (SEIRA) are techniques that have been studied in this regard. SEIRA shows a noticeable enhancement of molecules in the mid-infrared excitation on nonmetallic substrates.

Research Aim: The aim of this study was to develop a method for the detection and identification of trace levels of 3,4-methylenedioxymethamphetamine (MDMA) using gold nanoparticles (AuNPs) substrates with SEIRA. The objective was to address the current issue of misuse and addiction to drugs, especially methamphetamine and its derivatives.



Methodology: The researchers prepared AuNPs and mixed them with different concentrations of MDMA samples. The substrate was fabricated by mixing the AuNPs and MDMA samples, followed by vigorous stirring to allow molecules to be adsorbed on the AuNPs. This rigorous approach resulted in remarkable SEIRA, even at trace levels of MDMA.

Findings: The research demonstrated that the developed method using AuNPs substrates with SEIRA was able to detect trace levels of MDMA with high sensitivity. The approach showed rigidity, providing a reliable method for the detection and identification of drugs.

Theoretical Importance: The study highlights the potential of SEIRA for the characterization and identification of adsorbed molecules on metallic surfaces, particularly at trace levels. The sensitivity of SEIRA was found to be up to 50 times higher than the IR reflection-absorption spectroscopy (IRAS) technique commonly used for measuring IR spectra of adsorbed molecules on metallic surfaces.

Data Collection and Analysis Procedures: The researchers collected data by preparing AuNPs substrates and mixing them with MDMA samples of different concentrations. The SEIRA measurements were performed following the fabrication of the substrate. The analysis involved observing the enhancement and detection of trace levels of MDMA using SEIRA.

Question Addressed: The main question addressed in this study was whether trace levels of MDMA can be detected and identified using AuNPs substrates with SEIRA. Additionally, the researchers aimed to determine the sensitivity and efficiency of SEIRA compared to traditional IRAS techniques.

Conclusion: The study successfully developed a simple and highly sensitive method for the detection and identification of trace levels of MDMA using AuNPs substrates with SEIRA. The method proved to be cost-effective and highly selective. It has the potential for routine tests to obtain high-quality results with proper accuracy. This research significantly contributes to the field of drug detection and identification, especially in the case of methamphetamine and its derivatives.

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O29. Doping vs Functionalization: advanced modification strategies for enhanced sonophotocatalytic degradation of contaminants of emerging concern from water

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The presence of contaminants of emerging concern, such as pharmaceuticals, in wastewater poses significant risks to both human health and ecosystem biodiversity, due to their persistence, bioaccumulation, and potential to disrupt biological processes [1]. Therefore, there is a pressing need for advanced materials with enhanced properties to face the resilience of these contaminants.

Bismuth sulphur iodide (BiSI) has unique optical properties, high chemical stability, and excellent sonocatalytic activity, making it a promising material for the degradation of organic contaminants [2]. However, its narrow bandgap results in rapid electron-hole recombination, limiting its stability and efficiency under visible light irradiation. Consequently, modifications are required to improve its catalytic performance and extend its practical applications.

In this study we explore four different modification strategies of BiSI: (i) structural doping with oxygen to introduce sulphur vacancies and enhance the carrier separation and transfer; (ii) surface doping with silver ions, improving the visible light absorption; (iii) functionalization with graphene oxide (GO), aiming to increase the surface area for contaminant adsorption; (iv) functionalization with carbon nitride (C₃N₄), aiming to boost the photocatalytic activity [3].

All composites were fully characterized in terms of structural, physico-chemical, and optical properties, and applied on the degradation of carbamazepine (CBZ) via photocatalysis, sonocatalysis, and a combined sonophotocatalytic method. All the modified materials showed improved degradation efficiency across all methods. Using the combined sonophotocatalytic approach under ultrasound and visible light irradiation, degradation efficiencies of 58, 73, 85, 86, and 91% were obtained for BiSI, O-BiSI, C₃N₄@BiSI, Ag@BiSI, and GO@BiSI, respectively. The modifications were deeply investigated to uncover their effect on the properties and performance of the composites. Plausible degradation mechanisms were proposed for all materials, highlighting the impact of each modification on the generation of reactive species and consequent degradation pathways. These findings underscore the effectiveness of the proposed modification strategies in enhancing the properties of advanced materials, offering a sustainable and green approach for removing carbamazepine from water.

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O30. Enhancing efficiency of solid oxide electrolysis cells through carbon-assisted approach: Materials characterization and performance analysis

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Solid oxide electrolysis cells (SOECs) have garnered significant attention as an efficient means of producing green hydrogen using renewable electricity. The conventional SOEC design can be enhanced by supplying carbon-based depolarizing agents such as hydrocarbons, biogas, or coal, to the cathode compartment. This approach offers a reduction in the overall energy consumption required for steam electrolysis, a crucial factor in lowering the cost of hydrogen production. This study aimed to explore the utilization of solid carbon as a depolarizing agent for carbon-assisted solid oxide electrolysis cells (CA-SOECs) and focused on the characterization of selected anode materials and analysis of factors influencing the cell performance such as temperature, gas composition and flow rates, current density, and operating voltages.

The experimental setup comprised a button-size electrolyte-supported electrolysis cell with an anode chamber containing solid carbon mechanically attached to the anode surface. Three different compositions, $\text{Sr}_{0.7}\text{Ce}_{0.3}\text{MnO}_{3-\delta}$, $\text{SrFe}_{0.75}\text{Mo}_{0.25}\text{O}_{3-\delta}$, and $\text{Pr}_{0.15}\text{Sr}_{0.85}\text{TiO}_{3-\delta}$ were examined as potential candidates for anode material. The obtained experimental dataset includes the electrochemical impedance spectroscopy results and voltametric characteristics of the model electrolyzer under different operation conditions.

The results contribute to a deeper understanding of CA-SOEC performance and critical factors responsible for efficiency and stability of operation. Post-mortem analysis revealed that $\text{Sr}_{0.7}\text{Ce}_{0.3}\text{MnO}_{3-\delta}$ electrode is unsuitable for carbon-assisted SOECs due to reductive degradation in contact with carbon. On the other hand, $\text{SrFe}_{0.75}\text{Mo}_{0.25}\text{O}_{3-\delta}$ demonstrated appropriate stability under operating conditions and was identified as a promising electrode material for CA-SOEC applications.



O31. Laser Floating Zone as a tool for high temperature SrTiO₃ and TiO₂-based oxide thermoelectrics

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The increase in energy consumption is expected to continue, and the need for renewable and efficient energy sources is imperative [1]. Thermoelectric (TE) energy harvesting is a promising solution to reduce heat loss in high-temperature industries, using heat harvesting as a potential solution [2]. Still, “traditional” TE are not capable of resisting high temperatures and/ or harsher environments; thus, suitable and high performing TE materials are needed [3].

Oxide TE are usually characterized for their high chemical and thermal stability and are a prime candidate for this type of applications [4]. Nonetheless, most oxides are not suited for TE heat harvesting, with low ZT values when compared with traditional TE. Nevertheless, designing new compositions and micro-/nanostructures, as well as, involving new processing techniques can lead to unique microstructural and electrical properties, resulting in increases in TE oxide performance [5]. Promising families of oxides for TE applications like the titanates, namely SrTiO₃ and TiO₂, are sensitive to redox and processing conditions, resulting in flexibility towards tuning their electrical properties [6,7].

The present work focuses on a new approach for processing SrTiO₃ and TiO₂ -based TE materials, using the Laser Floating Zone (LFZ) technique. This technique provides various advantages for TE applications, including uniform distribution of the cations composition in the melt, tunable phase formation and cation distribution controlled by the cooling rate and high density, while also producing reducing conditions during LFZ processing [6]. Analysis and characterization of relevant effects of LFZ processing on the structure, microstructure and thermoelectric performance of the SrTiO₃ -based and TiO₂ -based materials are shown in this study. Results show the ability to prepare mechanically strong fibres with adequate electrical and TE properties, using LFZ. After LFZ processing, an annealing was also employed in selected samples, revealing a considerable improvement in electrical conductivity and high power factor values, related with the further reduction and charge carrier generation, as well as phase stabilization.

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O32. Enhancing Electrical Properties of Barium Titanate-Based Ceramic Thermoelectrics: Comparing Solid State Technique and Spark Plasma Sintering

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Ceramic thermoelectric materials are increasingly important due to their applications in energy conversion and waste heat recovery. The synthesis and sintering methods used significantly affect their properties and performance. This study examines the electrical properties of Barium Titanate-based thermoelectric materials using two common techniques: the solid-state method and spark plasma sintering (SPS) [1][2][3].

In the solid-state technique, samples are pressed uniaxially and then subjected to cold isostatic pressing (CIP). In contrast, the SPS method involves directly placing powders into a graphite die for simultaneous pressing and sintering without pre-pressing. After sintering, phase identification was carried out using powder X-ray diffraction (XRD), and morphological and microstructural characteristics were analyzed using scanning electron microscopy (SEM) with energy-dispersive spectrometry (EDS) for elemental analysis. The densities of the sintered samples were measured using the Archimedes method to ensure accuracy. Electrical conductivity and the Seebeck coefficient were measured simultaneously using a four-point probe DC method.

The results indicated that charge carrier transport was primarily controlled by electrons, as evidenced by the negative Seebeck coefficient across all temperatures, indicating n-type behavior. Notably, samples sintered via SPS exhibited a substantial increase in electrical conductivity—approximately three times higher at high temperatures and six times higher at low temperatures—compared to those sintered using the solid-state method. Consequently, the Power Factor improved significantly, by nearly ten times at lower temperatures and three times at higher temperatures, when sintered using SPS.

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O33. Biogas conversion system for green liquid fuel production

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Introduction – growing energy demand, particularly in the transportation sector, presents the need to explore new synthetic routes to produce renewable liquid fuels that can reduce pollution and carbon emissions to reach the net-zero target [1]. Biogas is a promising renewable energy source that can be used for the production of liquid fuels while significantly reducing greenhouse gas (GHG) emissions derived from the transportation sector [2]. The biogas composition consists mainly of CH₄ and CO₂ depending on the feedstocks. Other minor components include H₂S, H₂O, N₂, O₂, H₂, NH₃, siloxanes, and aromatics [3]. Large-scale biogas plants are a viable source for the efficient conversion of CH₄ and CO₂ into high-value products. There are various current options for biogas utilization, such as the biogas can be upgraded to biomethane and be used to supplement natural gas. Nonetheless, these routes are not without their challenges.

Challenges - The major challenges in biogas utilization for high-value products such as transportation fuels are its purity level, fluctuations in gas composition and flow rate, and low energy efficiency and productivity as compared to equivalent fossil fuels [4].

Solutions and discussion – To overcome these challenges, the current study suggests focusing on the route of biogas conversion to liquid fuel. This route aims at converting biological resources into liquid fuels with a high calorific value that can replace fossil fuels such as gasoline or diesel. This pioneering, but undeveloped, path first involves converting the biogas feedstock into synthesis gas (CO and H₂), which is further converted into synthetic green liquid fuels via the Fisher Tropsch synthesis process (FT). The biomass-to-liquid process has four basic stages: (1) transport and pre-treatment of biomass, (2) synthesis gas production, (3) Fischer-Tropsch synthesis, and (4) upgrade of FT liquids to high-quality fuels.

The main obstacles that prevent its commercialization are the high costs of transporting and preparing the biomass, stage (1), and the high FT plant capital costs, stage (3) [5]. However, the costs associated with the stage (1) can have diminished impact if higher energy-density fuels can be produced, at source. In this respect, the FT process selectivity must be improved to make downsizing and distributed production profitable [6]. The FT process is highly dependent on the local H₂/CO ratio on the catalyst, the residence time, the temperature, and pressure [6]. For this reason, the process can be highly successful in tailoring the products to the desired fractions by controlling local concentrations of H₂/CO and temperatures in the reactor [7]. However, the challenge remains for separating the synthesis gas precursor into its constituent fractions (i.e., CO and H₂), a task which is currently performed by oscillation adsorption of multicycle pressure. The current study proposes a more energy-efficient solution to resolve this impasse by creating a new electrochemical method using a proton-conducting ceramic membrane to instantly separate the H₂ and CO products needed for the distributed supply of the FT feeding [8]. This may provide a paradigm shift in these processes, by taking



advantage of the biogas as a non-primary and sustainable source of energy, where its high CO₂ content lends itself to the CO₂/CH₄ reforming.

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O34. The Influence of T-Shape Flow Deflector Placement on Convection Heat Transfer over an Array Heated Blocks

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In this study, a numerical exploration is conducted to investigate the convective heat transfer within a horizontal channel containing multiple heated blocks. The channel configuration integrates T-Shape flow deflectors strategically positioned downstream of each block. Air, characterized by a Prandtl number of 0.71 and possessing constant thermal properties, is utilized for cooling within the system. The geometric attributes and arrangement of the flow deflectors remain consistent throughout the analysis. The computations are centered around a Reynolds number of 400, while the positions of the flow deflectors are systematically varied. The finite volume method, implemented via Ansys Fluent © software, is employed to numerically solve the governing mathematical equations. The findings underscore a significant impact stemming from adjustments to the flow deflector configuration, influencing not only the fluid flow patterns but also the heat transfer characteristics across the heated blocks



Poster presentations



P1. Numerical study of the mechanical behaviour of concrete with polypropylene fibre

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To improve the mechanical characteristics (compression and tensile) of concrete, polypropylene fibres are added. And already known, concrete is the most used building material in the world. It is a heterogeneous composite material composed of a large granular skeleton (from micron to several tens of millimeters) coated by a porous matrix constituted by the hydrated cement paste. The aim of this work is the study of ordinary concrete at mesoscopic scale. and particularly study the effect of the Interfacial Transition Zone and the influence of the matrix (cement)/fibre (polypropylene) interfacial on the mechanical behaviour of concrete. based on digital tools (abaqus).

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P2. Photodegradation of Methylene Blue by CeO₂/NiO Modified Silicon Nanowires

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In this work is to deposition of CeO₂/NiO on SiNWs which present a high specific surface and to evaluate its catalytic activity for the degradation of blue methylene (BM) under Visible light irradiation. The silicon nanowires were elaborated by metal assisted chemical etching and the Cerium and Nickel was deposited by methods Hydrothermal. The samples were analyzed by scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX). The samples showed a high efficiency for the BM photodegradation especially, under visible light irradiation where a degradation rate of 98% was obtained after 90 min.



P3. Photoelectrochemical Conversion of CO₂ using HCl-PANI/Cu Photocathode

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The present study was aimed to convert CO₂ into value-added products such as methanol which not only could address the potential solution for controlling the CO₂ concentration level in the atmosphere but also can offer an alternative approach for the production of renewable energy sources. Photoelectrochemical reduction of carbon dioxide to value-added products and fuels is a promising and current method. In this perspective, Polyaniline (PANI) thin films were successfully synthesized using the electrodeposition technique from a mixed solution of 0.2M aniline and 0.5M HCl on copper. The morphological characterizations of the hybrid photoelectrocatalysts with or without sensitization with copper oxide (Cu₂O) particles were carried out by Scanning Electron Microscopy (SEM), while the catalytic activity was studied by linear sweep voltammetry (LSV) in dark and under white light irradiation using potentiostat station. Cyclic voltammetry in presence and without purging CO₂ was also conducted.

It was observed that the combination of PANI and copper (I) oxide greatly increased PEC carbon dioxide reduction to methanol owing to the enhancement in the carbon dioxide chemisorption capacity by the photocathode surface. Gas chromatography (GC) showed a concentration of 27% corresponding to methanol production, when the copper (I) oxide/PANI/Cu heterostructure was used as a photocathode compared to the unmodified which exhibit 25%, at an applied potential of -1.2 V. From the obtained results, Cu₂O/HCl-PANI/Cu could be useful as a promising candidate for the CO₂RR to Methanol.



P4. Impact of silicon surface modification on the catalytic performance towards CO₂ conversion of Cu₂S/Si-based photocathodes

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In order to prevent global warming, which is mainly caused by the increase in carbon dioxide level in the atmosphere, it is interesting to produce renewable energy in the form of chemical energy by converting carbon dioxide into alternative fuels and other energy-dense products. Photoelectrochemical reduction of carbon dioxide to value-added products and fuels is a promising and current method. The objective of our study is to develop Cu₂S-based photoelectrodes, in which Cu₂S is used as CO₂ photoelectrocatalyst deposited on nanostructured silicon substrates. Cu₂S thin layers were deposited using the chemical bath deposition (CBD) technique. Silicon nanowires and nanopillars were obtained by alkaline etching. SEM and UV-visible spectroscopy were used to analyze morphology and optical characteristics. By using a potentiostat station, we characterized the photoelectrochemical properties. We performed cyclic voltammetry in presence and without CO₂ purging as well as linear voltammetry (LSV) in the dark and under white light irradiation. We perform chronoamperometry to study the stability of our photocathodes. The quality of the nanowires and nanopillars was visible in the SEM images, and after Cu₂S deposition, we could see how the deposition was distributed over the textured surfaces. The inclusion of the Cu₂S layer applied on textured substrates significantly reduces the reflectance (R%). The catalytic performance towards CO₂ conversion of Cu₂S/Si-based photocathodes revealed that the texturing of the silicon surface with nanowires and pillars have a better photoelectrochemical behavior than those without surfaces modifications.



P5. The Properties of lightweight artificial aggregates from construction waste

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The article will present a description of the technology for producing lightweight artificial aggregates from construction and industrial waste, the problem of its management occurring in Poland, most countries and the European Union. The basic parameters of the obtained lightweight aggregates are also presented: density, compressive strength and frost resistance. The chemical composition and leachability of hazardous substances were also analyzed. Environmentally friendly production technology parameters were proposed. The obtained results allowed for the issuance of recommendations regarding the use of aggregates in construction and other industries. This experimental work shows the example of recycling construction waste and circular economy policy.

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P6. A biocompatible acrylic resin with solvent as a potential material for obtaining microneedle transdermal systems using masked stereolithography

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One direction in the development of materials science within the pharmaceutical industry is the design of solutions to personalize treatment methods for patients [1]. Microneedle transdermal systems (MTSs) allow drug delivery through the skin in controlled way. Additive methods are feasible for MTSs manufacturing, allowing the production of parts with complex geometries, like microneedles, generating negligible waste products. One variety of MTSs is hydrogel-type system, which relies on drug loading of the MTS and diffusion of the drug through the structure of the matrix material into the human skin through pores in the *stratum corneum* formed by the mechanical action of the microneedles [2]. Drug loading of the matrix material often requires the use of additional processes or substances, including solvents and cosolvents [3]. In order to increase the application potential of additive methods in MTSs production, the effect of ethanol, used as a solvent for active pharmaceutical ingredients and cosolvent in the process of dissolving drugs in resin, on the properties of biocompatible acrylic photo-curable resin parts obtained by masked stereolithography was studied. Samples made of resin and resin with the addition of alcohol at concentrations of 15%, 25% and 35% were obtained and studied. The effect of ethanol on tensile strength and changes in geometric dimensions of the samples was determined. Deterioration of properties caused by the presence of alcohol was observed, as well as an intensification of the changes with an increase in alcohol concentration, which is most likely due to the effect of the solvent on the UV light-induced radical polymerization of the resin. The conducted studies made it possible to determine the optimal ethanol content, which still allows the obtained system to be potentially used as a matrix material for microneedle transdermal systems and significantly increases the maximum amount of drug that the matrix can potentially be loaded with. The obtained results make an important contribution to the state of the art and the applicability of acrylic biocompatible photoresins in the process of obtaining MTSs.

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P7. The Properties of cement composites with lightweight artificial aggregates produced from construction and industrial waste

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The article will present the properties of artificial aggregates made from construction and industrial waste according to our own technology. Additionally, these aggregates were used to produce lightweight concrete. Based on the planned experiment, basic tests were carried out on the physical and mechanical properties of mixtures and concretes, such as: consistency, density of the concrete mixture, compressive and bending strength after 14 and 28 days of curing, water absorption, bulk density, thermal insulation. Environmentally friendly production technology parameters were proposed. The obtained results allowed for the issuance of recommendations regarding the use of aggregates in construction and other industries. This experimental work shows an example of construction waste recycling and circular economy policies.

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P8. Preparation and characterization of Al alloys modified by the addition of Re for Spark Plasma Sintering

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Over the last few decades, Al alloys have been increasingly exploited for industrial applications, especially in the aviation, automotive, or construction sectors [1]. Despite their favorable properties, such as low density, there are still some limitations associated with their mechanical or anticorrosive properties. Therefore, with the aim of improving these aspects, powder modification is often employed [2]. In this research, the attempt for the Al7050 and Al7075 alloys reinforcement with the addition of various contents of Re (0.5÷3 wt%) is presented. The powder samples of the Re-modified Al alloys were prepared by ball-milling in a planetary mill. First, phase composition was tested via X-ray diffraction analysis. The effects of Re content on the physical properties of the powders were investigated. Apparent density and specific surface area were determined using the gas pycnometry method and gas adsorption measurements, respectively, and based on their results, average particle size was determined. Moreover, particle size distribution by the laser diffraction method was performed. It was shown that with increasing Re addition, density and specific surface area of the samples are increased. The prepared powders exhibited an even particle distribution after the milling process. Discussed materials will then be used as raw material for the fabrication of sinters via Spark Plasma Sintering technology. Despite the difficulties in processing Al alloys with the addition of Re, related primarily to considerable difference in the melting points of the discussed materials, our further research will answer the question of whether such modifications have a beneficial effect on the mechanical properties of Al alloys.

Acknowledgments

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P9. Application of semiconductor-based APS coatings for the light-activated decomposition of persistent organic pollutants

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Constantly increasing environmental pollution levels entailed a strive to find effective, accessible, and cost-effective methods for the removal of harmful substances from soil and water [1]. Among the various proposed solutions, the development of photocatalytic coatings is one of the most important directions for the advancement of environmental protection [2]. The presented work focuses on the research on photocatalytic removal of organic pollutants from aqueous solutions by glass-ceramic coatings fabricated via atmospheric plasma spraying technology (APS). Powder samples of nanometric TiO₂ and Al₂O₃ or SnO₂ and ZrO₂ were granulated with a polyvinylpyrrolidone and applied as a feedstock material in the APS process. Two types of binary coatings – TiO₂/Al₂O₃ and SnO₂/ZrO₂ – with contents of oxides variable at every 15 wt%, were obtained. Chemical and phase composition were examined using XRD analysis. Morphology and the elemental distribution on the surface of coatings were analyzed by SEM observations and surface profile parameters were determined by roughness measurements. Organic compounds catalytic degradation ability by the coatings was determined in the process of UV-light activated decomposition of Eosin Y (Eo) from an aqueous solution (cont. 5 mg/L). Color measurements before and after the reaction were also done using a sphere spectrophotometer in CIELab color space. The efficiency of Eo removal varied and its lowest values were stated at 22% and 37% for 100 wt% ZrO₂ and 15 wt% TiO₂ coatings. The greatest effectiveness – 71% and 65% – was achieved by 100 wt% TiO₂ and 100 wt% SnO₂ coatings, respectively. Results indicate that the fabricated coatings have a great potential for application in persistent organic compounds degradation in wastewater treatment processes.

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P10. Physical and mechanical properties of mortars with synthetic zeolites

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The correct selection of the characteristics of a restoration plaster system can be crucial to the success of restoration work [1]. The aim of this study was to design and test the properties of restoration plaster with zeolite cement. The used zeolites (ZSM-5, Na-A) were characterised by different Si/Al ratio. Zeolites proved to be an ideal additive for restoration mortars due to their porous structure. The mortars were characterised by higher porosity, absorbability, frost resistance, resistance to salt crystallisation pressure and strength compared to a reference mortar with pure CEM I 52.5R cement [2]. The mortars with the high-silicon zeolite ZSM-5 showed the best properties. The 35% addition of zeolite to the cement increased the strength of the mortars by 10.5% compared to the reference mortar (4.3 MPa). The best results in the frost resistance test were also obtained by the plasters with the addition of zeolite ZSM-5. The weight loss in this case was: ZSM5 15% - 0.03%, ZSM5 - 35% - 1.79%. The results are related to the amount of active SiO_2 and Al_2O_3 in the crystal structures of the zeolites. The oxides react with $\text{Ca}(\text{OH})_2$ to form a C-S-H phase responsible for the high strength [2,3]. The higher amount of active silica and the higher Si/Al ratio resulted in the C-S-H phase being more.

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P11. Influence of firing temperature on the properties of eco-friendly lightweight aggregates

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Abstract: The lightweight aggregate was obtained from reservoir sediments, municipal from incineration bottom ash, construction debris, clay and alkali additives. After complete drying, they were fired at 1000°C and 1050°C for 30 minutes. The increase in firing temperature increases densities of aggregates. Aggregates sintered at 1000°C reached a value of particle density of 1.70 g/cm³, loose bulk density of 0.811 g/cm³, while those sintered at 1050°C reached a value of particle density of 1.98 g/cm³ and loose bulk density of 0.984 g/cm³. The water of absorption of aggregates sintered at a higher temperature is 14%, while at a lower temperature it is 1.5% higher. Aggregates sintered at 1050°C have a compressive strength three times higher than those sintered at a lower temperature.

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P12. Influence of low-silicon and high-silicon zeolite addition on changes in the microstructure of pastes

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Globally, cement production has a negative impact on the environment. This is related to the use of a huge amount of geological natural resources in the form of limestone rocks, and the emission of a large amount of CO₂ into the atmosphere [1]. The production of one ton of this raw material, is associated with the emission of 0.5-1 ton of carbon dioxide into the atmosphere, as well as a huge consumption of energy, which causes significant environmental pollution. Recently, investigators have been looking for mineral additives to cement that could partially replace it and at the same time improve the physical-mechanical parameters of pastes, mortars or concretes [2].

In the present study, the effect of the addition of zeolites (high-silicon and low-silicon) on the process and products of cement hydration was investigated. For the purpose of achieving the stated goal, components of the allite-zeolite system were obtained by synthesis. The effectiveness of the synthesis was evaluated on the basis of chemical and phase composition analysis and textural studies. The effect of pozzolanic additives on the hydration process was evaluated by XRD analysis, SEM, microcalorimetric and conductometric studies. Cement paste with 15%, 35% and 50% zeolite additives were analyzed after 7, 28 and 90 days of curing. The results showed that each amount of additive reduced the heat release rate and total heat of hydration. The hydration products formed are affected by the curing time and the type of zeolite. The use of zeolite additive in the right amount in the production process of cementitious composites can positively affect its physical and mechanical properties. Zeolites reduced the ratio of CaO/SiO₂ in the C-S-H phase, which for pastes with the addition of the Na-A ranged from 1.61 to 1.37, and for the ZSM-5 from 1.91 to 0.47. This ratio changed with the amount of addition and the maturation time of the pastes.

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P13. Rejuvenating agents of waste origin used in the mix asphalt with RAP

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In recent years, accelerated degradation of road pavements and increasing the amount of reclaimed asphalt pavement (RAP) has been a major problem occurring in many countries. On the other hand, the use of reclaimed asphalt pavement in the asphalt mix is limited due to the altered properties in the aging process of the asphalt. In order to improve the mechanical properties of asphalt mix containing RAP it is necessary to use either softer binder, rejuvenators or bitumen modified with synthetic polymers, while limiting the asphalt aging process is possible through the use of warm mix asphalt technology.

This paper presents an evaluation of the properties of zeolite foamed asphalts with used waste engine oil (WEO). In this research, synthetic zeolite NaP1 and natural clinoptilolite soaked with water were used. On the basis of tests of properties of asphalts (dynamic viscosity and penetration) with WEO and zeolites in concentrations of 0, 3, 5, 7%, the optimal amount of zeolite material was determined. Then, water and frost resistance of the asphalt mixture with 20% addition of RAP was determined. The results of testing the properties of bitumen with the addition of zeolites and WEO in various proportions are presented in tab. 1.

Table 1. The results of viscosity tests for 20/30 asphalt with the addition of WEO and zeolites.

addition	7% NaP1	5% NaP1	3% NaP1	7% CLIN	5% CLIN	3% CLIN
Viscosity [mPa·s]						
7% WEO	209	211	212	210	191	179
5% WEO	250	245	231	244	235	236
3% WEO	292	289	274	275	274	267
Penetration [0,1 mm]						
7% WEO	49.0	48.2	47.5	44.0	40.4	44.7
5% WEO	37.5	37.0	36.9	36.5	37.8	35.9

The viscosity of the 20/30 asphalt was 377 mPa·s. Viscosity decreased as the WEO addition increased. The highest percentage change of viscosity was observed with 3% added WEO. Simultaneously, in samples with zeolite materials, the viscosity increased. The test results also indicate a significant increase in the penetration of asphalt with the addition of WEO. The asphalt binders foamed with zeolites had slightly lower penetration. This is caused by the effect of bitumen stiffening after adding a solid in the form of dust. Based on the results of bitumen viscosity and penetration tests, a 7% additive calculated for the weight of bitumen contained in the RAP was used in the tests of asphalt mixtures.



P14. Study of the antibacterial effect of fluorohydroxyapatite combined with ginger oil extract

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Hydroxyapatite (HAp), with good mechanical properties, is a promising material for a number of useful applications in dentistry and orthopedics, as well as in biomedical engineering for drug delivery, filling of bone defects, bone cements, etc. Fluorine-doped hydroxyapatite (FHAp) is primarily intended for application in dentistry thanks to the properties of fluoride for oral health. It contributes to the mineralization of dental enamel and prevents the formation of dental caries. During this work, initially, HAp and FHAp were synthesized by precipitation. Characterization is done by Fourier transform infrared spectrometry (FTIR), X-ray diffraction (XRD), thermogravimetric analysis (TGA). Secondly, fluorohydroxyapatite was the subject of a study of its antibacterial properties on the bacterial strains *Staphylococcus aureus* and *Escherichia Coli*. The test consists of carrying out an antibiogram by diffusion in agar medium (disk method). A second test was carried out by coupling the effect of FHAp with an extract of ginger essential oil obtained by maceration. According to the results obtained from the antibiogram, we see that FHAp has no antibacterial effect on the bacterial strain *Staphylococcus aureus* and *Escherichia Coli*. The FHAp test with ginger essential oil shows a certain antibacterial effect on both bacterial strains.



P15. Multiscale studies of electric micropropulsion for small spacecraft

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With the advent of microelectromechanical systems (MEMS), reduced satellite size and mass has led to lower launch costs, enabling the use of satellite constellations and space-based educational platforms. Electric propulsion is highly efficient for both deep-space and near-earth applications and it is an excellent candidate for small satellites. An electrospray electrostatic thruster for small spacecrafts is discussed in the present paper. Electrosprays and field-emission electric propulsion, which use ion sources, are promising for small spacecraft given that their performance increases at the microscale. A multi-scale approach (encompassing several scales of modelling: fluid, particle trajectory, electric field and molecular modelling) is adopted in order to gain an increased understanding of complex underlying physical processes. The governing factors are accessed in order to obtain the onset and maintenance of a focused beam. The multi-scale results has the potential of providing valuable insights for the design and characterization of a laboratory model of an electrospray micro-propulsion system for small spacecrafts. The prototype thrusters described in this research will demonstrate how various electric propulsion systems [1-3] could be combined into a multimodal system to provide effective thrust for small spacecraft.

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P16. Tunable Raman features in nanomaterials belonging to Nb₂O₅-SiO₂, binary oxide systems

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-Abstract

Raman scattering in transparent glass-ceramics (TGCs) based on Nb₂O₅-SiO₂, binary oxide systems were investigated with the aim to explore the influence of micro- and nanoscale structural transformations on Raman gain.

-Introduction

Nonlinear conversion is a fundamental aspect of nonlinear photonics, allowing the realization of efficiently integrated coherent light sources. Several second and third order nonlinear optical phenomena (among which Stimulated Raman Scattering) can be involved. Among the nonlinear nanostructured materials, transparent glass-ceramics (TGCs) play a key role, due to their nonlinear optical features, which can be finely tuned by suitable chemical and heat treatments [1].

-Results

Nanostructured TGCs were synthesized, starting with 8BaO·15Na₂O·27Nb₂O₅·50SiO₂ (BaNaNS) glass, by proper nucleation and crystallization heat treatments. TGCs are typically composed of nanocrystals, uniformly distributed in the residual glass matrix, with a variable crystallinity degree. A significant Raman gain improvement for both BaNaNS glass and TGCs with respect to SiO₂ glass is demonstrated, which can be clearly related to the nanostructuring process [2].

-Discussion

These findings show that the nonlinear optical functionalities of TGC materials can be modulated by controlling the structural transformations at the nanoscale rather than microscale.

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P17. Statistical Tolerance Synthesis based on Jacobian Torsor Model and form deviations in mechanical assemblies

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The purpose of this communication is to conduct a theoretical and practical study that aims to illustrate the influence of form deviations on mechanical assemblies. This study presents a statistical approach for redefining tolerances by combining the Jacobian torsor model and Monte Carlo simulation. The first step in this method is to identify the functional requirement of the assembly and then the functional elements in the tolerance chain. Once these elements are defined, the Jacobian Torsor model can be constructed to describe the functional relationship between them. The process involves redistributing the tolerances until the functional need is consistent with the provided functional requirement. The results demonstrate that this method is a practical way to redefine statistical tolerances. Finally, through a comparative study, the results prove the performance of the proposed approach.



P18. Anelasticity, internal friction in radiation and structural functionalized nanocomposites of multiwalled carbon nanotubes and polyamide, polyethylene, polyvinylchloride, SiO₂

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Abstract

Anelasticity, internal friction (IF) Q^{-1} in radiation functionalized nanocomposites of polyamide, polyethylene, polyvinylchloride, SiO₂ and multiwalled carbon nanotubes (MCNT) is represented.

Introduction

Mechanical characteristics of nanocomposites based on polyamide, polyethylene, polyvinylchloride with MCNT, in which atoms number on the surface is compared to the total atoms number, the dimensions of which at least in one direction, range from several to hundreds nm, fundamentally differ from mechanical characteristics of macroscopically homogeneous systems.

Experimental Methods

Ultrasound (US) impulse-phase method using computerized “KERN-4” with frequencies $f_{\perp} \approx 0,7$ MHz and $f_{\parallel} \approx 1$ MHz was used [1-3]. The measured velocity error was equal to $\Delta V/V \approx 1,5\%$. The samples were prepared by ultrasonic dispersion using digital US bath CE-6200A with power $W = 70$ W at frequency $f \approx 42$ kHz.

Results and Discussion

Illustrations of the window for processing data of quasilongitudinal elastic waves velocity measuring $V_{\parallel} = 3244 \pm 10$ m/sec m/sec in nanocomposite polyamide (PA-6) $(NH(CH_2)_5CO)_n + 0,1\%$ MCNT by pulse-phase US method at frequency $f_{\parallel} \approx 1$ MHz after electron irradiation with dose $D_{e-} \approx 10$ MRad with energy $E_{e-} \approx 2,0$ MeV; in ZSh-35 are represented in Fig. 1, Fig. 2.

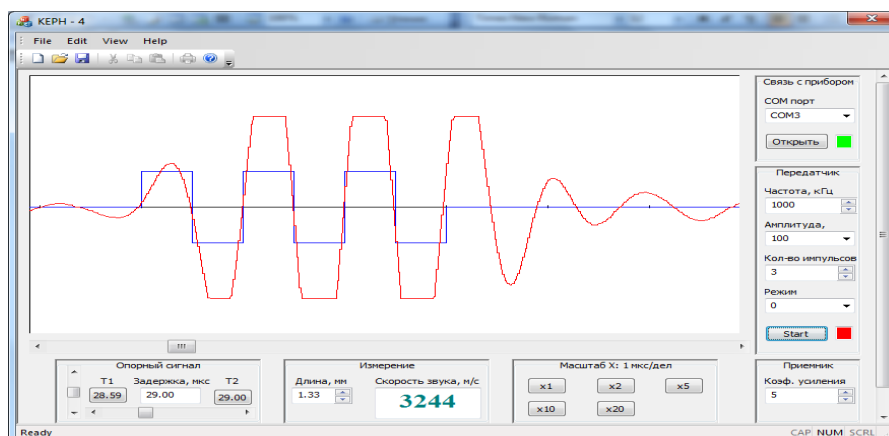


Fig.1. Illustration of the window for processing data of quasilongitudinal elastic waves velocity measuring $V_{\parallel} = 3244$ m/sec in nanocomposite polyamide + 0,1% MCNT after electron irradiation.

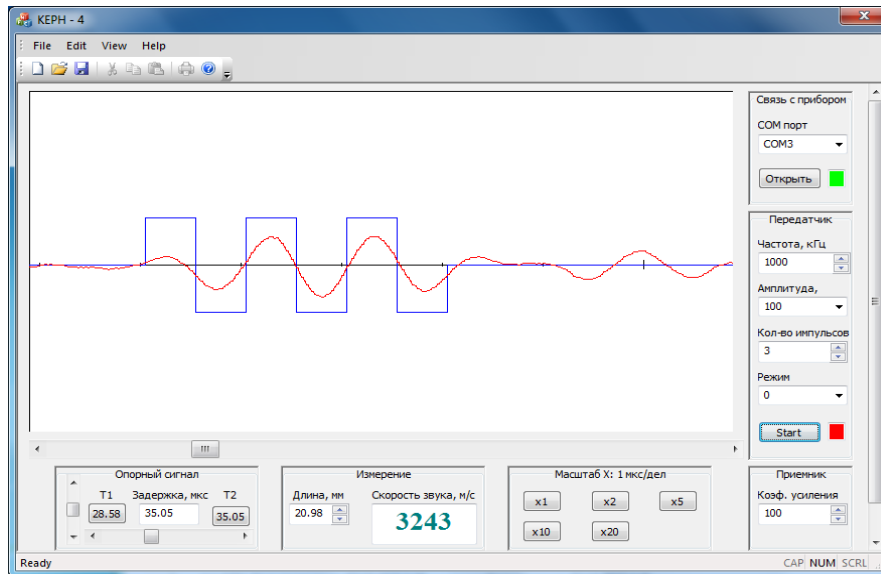


Fig. 2. Illustration of the window for processing data of quasilongitudinal elastic waves velocity measuring $V_{\parallel} = 3243$ m/sec in ZSh-35 by pulse-phase US method at frequency $f_{\parallel} \approx 1$ MHz.

Poisson coefficient μ and elastic modulus E completely characterize the elastic properties of polymer nanocomposite. Poisson coefficient μ - elastic value of ratio of relative transversal compression $\varepsilon_{\perp}$ to relative longitudinal lengthening $\varepsilon_{\parallel}$ and equal [1]:

$$\mu = -\frac{\varepsilon_{\perp}}{\varepsilon_{\parallel}} = -\frac{\frac{\Delta X}{X}}{\frac{\Delta l}{l}} = -\frac{\Delta X}{\Delta l} * \frac{l}{X}, \quad (1)$$

$$\mu = -\frac{\varepsilon_{\perp}}{\varepsilon_{\parallel}} = \frac{\frac{1}{2}V_{\parallel}^2 - V_{\perp}^2}{V_{\parallel}^2 - V_{\perp}^2} = \frac{1}{2} \left[1 + \frac{1}{1 - \left(\frac{V_{\parallel}}{V_{\perp}} \right)^2} \right]. \quad (2)$$

One oscillator produces 3 waves: 1 longitudinal and 2 transversal. Debye temperature θ_D was determined after the formula [2]:

$$\theta_D = \frac{h}{k_B} * \left(\frac{9N_A \rho}{4\pi A} \right)^{\frac{1}{3}} * \left(\frac{1}{V_{\parallel}^3} + \frac{2}{V_{\perp}^3} \right)^{\frac{1}{3}}, \quad (3)$$

where k_B - Boltzmann constant, h - Plank constant, N_A - Avogadro number, A - middle gram-molecular mass, $V_{\parallel}$ - quasilongitudinal US velocity, $V_{\perp}$ - quasitransversal US velocity.

Complex elastic modulus of nanocomposite polyamide-6 (PA-6) $(\text{NH}(\text{CH}_2)_5\text{CO})_n + \% \text{MCNT}$ E^* is equal to the sum of elastic dynamic modulus $E' = \rho V_{\parallel}^2$ and loss modulus $E'' = E' \delta$ [3]:

$$E^* = E' + E'' = E'(1 + \delta) = \rho V_{\parallel}^2 (1 + \delta) = \rho V_{\parallel}^2 (1 + \pi Q^{-1}) = \rho V_{\parallel}^2 \left(1 + \alpha \frac{V}{f} \right), \quad (4)$$

where δ - logarithmic decrement of US attenuation, ρ - nanocomposite density, $V_{\parallel}$ - longitudinal US elastic waves velocity, Q^{-1} - internal friction.

$$\frac{E''}{E'} = \delta = \pi Q^{-1} = \alpha \lambda = \alpha \frac{V}{f}, \quad (5)$$

where α - US attenuation coefficient, λ - US wavelength, f - US frequency. Internal friction is equal $Q^{-1} = \delta/\pi$. The logarithmic decrement of attenuation δ of US oscillations with amplitude $A = A_0 e^{-\delta x}$ is equal:



$$\delta = \ln \left(\frac{A_{n+1}}{A_n} \right). \quad (6)$$

Conclusions

1. The presence of the strong interaction for nanocomposite between polyamide-6 (NH(CH₂)₅CO)_n and multiwalled carbon nanotubes was confirmed.
2. The increase of the nanocomposite crystallinity degree at growth of multiwalled carbon nanotubes concentration filling with the nanotubes of matrix results in the decline of content of organized phase.
3. The phenomenon of change of Poisson coefficient μ , Debye temperature θ_D , dynamic elastic modulus $E' = \rho V_{\parallel}^2$, dynamic shear modulus $G = \rho V_{\perp}^2$ under the influence of radiative electronic e^- radiation is caused by the appearance of primary radiation defects (RD). As the result of interdefect interactions primary RD form secondary RD.

Acknowledgements

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P19. Local electromechanical properties of Glycine-Diphenylalanine tubes composites

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In the last decade, there has been enormous research interest in phenomena at the nanoscale, especially with the possibility of construction-controlled microstructure. The creation of micro and nanostructures from materials and composites with high values of important physical characteristics opens great prospects for controlling and enhancing these characteristics and, as a consequence, expanding the possibilities of their practical applications. We assumed that the high ferroelectric-piezoelectric activity of glycine and diphenylalanine nanotubes (FF-PNTs), which we had previously discovered, would also allow us to detect additional properties in their composites. Our assumption is based on the fact that glycine is a unique amino acid that contains hydrogen as a side chain (and not carbon, as in all other amino acids). Additionally, a unique property found in PNTs is the presence of subnanometer-scale crystalline regions, which may be responsible for many of the unusual properties of these materials.

Using Piezoresonance atomic microscopy (PFM) techniques, we investigated the mutual influence of PNT and glycine and demonstrate that ferroelectric behaviour can be modulated at the single-molecule level. Fine domain structure features in piezoresonance images were demonstrated to be related to the concentration ratio of glycine and FF PNT components responsible for the nanoscale mechanism of nucleation and growth of domains associated with defects.

Based on an analysis of the orientations of the polarization vectors of the nanotubes, we came to the conclusion that the nucleation of nanotubes occurs on the primary surface with opposite polarization directions at the nucleation sites. It was found that PNTs have a variable size along the growth axis and an abnormally small diameter at the tip.

The evolution of the domain structures of the glycine/FF PNT components with displacement indicated the presence of a well-defined threshold for the nucleation of ferroelectric domains and a gradual increase in domain size with displacement above this threshold, similar to PFM switching experiments in classical ferroelectrics materials. The measured piezoelectric coefficient (corresponding to the FF PNT over the entire glycine layer) turned out to be several times smaller than the value of pure FF PNT. This difference can be explained by specific microstructures with different glycine/FF PNT concentrations, which influence the effective piezoelectric coefficient.

This work was developed in the scope of the Project “Agenda ILLIANCE” [C644919832-00000035 | Project no. 46], financed by PRR – Recovery and Resilience Plan under the Next Generation EU from the European Union. This work also was supported, in terms of TEMA Research Infrastructure equipment, by the projects UIDB/00481/2020 and UIDP/00481/2020 - Fundação para a Ciência e a Tecnologia; and CENTRO-01-0145-FEDER-022083 - Centro Portugal Regional Operational Programme (Centro2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund.



P20. Development of thermoelectric composites with catalytic functionality

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The search for sustainable and cleaner energy is one of today's major concerns since the energy demand has achieved unprecedented values. Every day, large amounts of waste heat emitted by diverse processes are not being exploited, resulting in losses of 60% of the associated energy. This unused and cheap thermal energy is easily available and can be recovered. Thermoelectrics have emerged as a promising green technology to wisely take advantage and harvest this waste heat by converting it directly into electrical energy. This work aims to demonstrate a new concept of combining TE and catalytic functionalities in one system. The idea relies on the microstructural design of thermoelements with graded porosity, controlling the catalytic reaction rate and corresponding thermal effect. One of the challenges lies in the development of efficient microstructural architectures that incorporate both thermoelectric and catalytic functionalities while integrating multifunctional elements with graded porosity into a system capable of demonstrating a combined performance. In this work, a ceramics emulsification process was involved for processing strontium titanate-base ceramics with a designed porosity [1]. Following Taguchi approach, three variables with three levels were selected in the emulsification processing to evaluate the effects of amount of paraffin added as a pore former, surfactant concentration, and sintering temperature. Strontium titanate was selected as a model system, which can provide first processing guidelines for obtaining porous ceramics based on this material [2]. These guidelines will be further used for the preparation of novel composite materials containing Pr-substitutes strontium titanate as a matrix and MoNi_4 intermetallic micro- and nanoparticles, possessing combined thermoelectric and catalytic functionalities. Some preliminary results both on processing porous ceramics and thermoelectric performance of these new composites will be presented.

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P21. Effect of mechanical recycling on structural, mechanical and optical properties of high-density polyethylene (HDPE)

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The global plastic waste crisis has brought in recent years attention to the urgent need for the implementation of a circular plastics economy, in an ever-ending quest to maximize its value and lifespan. With technology progress in the production of polymeric parts using additive manufacturing, namely 3D printing, is an important factor to have in mind, and the use of recycled materials is a requirement in today's market. This study investigates the properties of high-density polyethylene (HDPE) during successive closed-loop mechanical recycling via multiple mixture and extrusion cycles. The main objective of this work is to perform a comprehensive study of the impact of the addition of carbon dots (CDs) on HDPE to improve the mechanical properties and optical traceability. The nanocomposites were prepared using different concentrations of CDs, by melt mixing followed by injection molding.[1] The mechanical, structural and optical characterization of the obtained nanocomposites was performed through X-ray diffraction (XRD), differential scanning calorimetry (DSC) stress/strain mechanical testing, among other techniques, to evaluate the effect of the CDs reinforcement on polymer's properties. For a 0.5% CDs concentration, an increase in tensile strength of 17% was verified after being recycled, with a strain at a maximum load of 11%, maintaining its crystalline nature, and showing a distinct optical signature. These preliminary results are good indicator of the potential of HDPE:CDs nanocomposites for application in additive manufacturing.

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P22. Two-dimensional conductive cobalt metal-organic frameworks for high performance supercapacitors

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Supercapacitors are electrochemical energy storage devices whose electrochemical performance depends on high porosity and conductivity characteristics. Metal-Organic Frameworks (MOFs) have recently got attention due to their very high porosity, high specific surface area (SSA), structure tunability, and multiple reaction sites. However, its low conductivity always limits its pristine usage as a high-performance electrode in supercapacitors. Therefore, in this work we have explored cobalt metal based two-dimensional conductive metal-organic frameworks (2DCMOFs) as a promising electrode material for high performance supercapacitors due to their large specific surface area, intrinsically prominent electrical conductivity, and plenty of functional groups for further bond formation. The one step stirring facile synthesis approach using deionized water is capable to form conductive 2D structures which is well confirmed by different structural and morphological characterizations. Therefore, we have prepared the electrode using as prepared 2DCo MOF and tested it in 1M H₂SO₄ electrolyte within a potential window of 0-1V. The as prepared pristine 2DCo MOF electrode delivers a high specific capacitance of 217 F/g at a current density of 1 A/g and extremely high volumetric capacitance of 658 F/cm³, which is much better than many non-conductive pristine MOFs. Therefore, this study opens new perspective for the performance enhancement of pristine MOFs based energy storage devices by generating the inherent conductivity.



P23. Microwave activated mixed biowastes derived porous carbon-based electrode for all-solid-state symmetrical supercapacitors

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Porous conducting carbons derived from several biowaste resources are gaining recent research attention as an electrode material for electrochemical capacitors. Herein, we have developed a highly porous carbon from mixed biowaste precursor (neem leaves, bamboo leaves and waste paper mixture in equal amount) using low power microwave oven in just 90 seconds. The microwave activation technique is fast, robust and low cost as compared to high temperature inert gas tube furnace-based technique. Furthermore, the as synthesized microwave derived carbon (MWDC) is used as an active electrode material for supercapacitors owing to its high porosity, high specific surface area and good conductivity. The as prepared electrode shows a high specific capacitance of 293 F/g at a current density of 1 A/g using 1 M H₂SO₄ aqueous electrolyte. Meanwhile, an all solid-state symmetrical supercapacitor is also assembled using two equally weighted MWDC electrode and PVA-1M H₂SO₄ polymer gel electrolyte. The 1.8 V MWDC//MWDC symmetrical solid-state device shows a very high energy density of 30.4 Wh/kg with a high-power density of 947.3 W/kg along with a long cycle life of 89.8 % after 2000 charge-discharge cycles. These remarkable results show a new pathway for the application of low cost biowastes derived activated carbon using low power microwave oven for next generation high performance alternative energy storage devices.



P24. Porphyrin – Based Carbon Dots for Photodynamic Therapy

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Introduction

Porphyrins present a high potential for biomedical applications including bioimaging, phototherapy and antibacterial. However, their low solubility in water has drastically hampered their use in biological environments. Carbon dots (CDs), which have excellent optical properties, good biocompatibility, and excellent water solubility, have emerged as interesting nanoplatforms for conjugation with porphyrins in order to increase their water solubility and consequently maximize their therapeutic effects. Although promising results have been achieved so far, it has been noticed that porphyrins tend to quenching with CDs, reducing their optical activity and ability to generate ROS. Furthermore, this conjugation usually tends to decrease CDs water solubility. Here we will explore the modification of porphyrin macrocycles with amine, hydroxyl and other functional groups capable of promoting their self-assembly into multifunctional CDs. With this approach we aim to obtain CDs that combine both the excellent optical and therapeutic activity of porphyrins, as well as excellent biocompatibility and water stability, giving rise to new theragnostic formulations.

Objectives

The objective of this project is to develop a new synthetic approach in which porphyrins will be explored as molecular precursors for CDs for cancer therapy.

Methods

The synthesis of porphyrin-based carbon dots (PCDs) will be based on the solvothermal method, using different porphyrins as precursors. Various reaction parameters will be explored to control the formation of PCDs.

The PCDs will be characterized using different solid-state spectroscopic techniques as Fourier transform infrared spectroscopy (FTIR), Raman, X-ray, photoelectron spectroscopy (XPS), transmission electron microscopy (TEM) and optical spectroscopy (UV-Vis absorption and fluorescence) in solution.

Discussion / Conclusion

With this new approach where porphyrin will be explored as molecular precursors of PCDs, it is expected to biologically improve their performance by increasing their solubility, optical performance and their ability to generate ROS species. This new PCD will play an important role in the development of highly effective theragnostic agents capable of providing effective fluorescent bioimaging monitoring and highly efficient photodynamic therapy. Ultimately, it is hoped that this project will drive the development of new PCDs, as well as theranostic agents, capable of successfully reaching pre-clinical testing.



P25. Enhanced Supercapacitor Performance with Redox Additive Electrolytes for UiO-66@ZIF-8 Material Study

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The integration of redox additives into aqueous electrolyte systems has garnered significant research interest for their ability to augment charge storage via additional redox reactions at the electrode/electrolyte interface. In this study, we investigate the electrochemical behavior of UiO-66@ZIF-8 core-shell metal-organic framework (MOF) based supercapacitors by incorporating Potassium Iodide (KI) as a redox additive in 1M H₂SO₄ aqueous electrolyte. The synergistic effect between KI and 1M H₂SO₄ enhances the reaction kinetics of the I₂/I⁻ redox pair and facilitates effective pore penetration through improved surface wettability, resulting in a notable increase in specific capacitance. Specifically, a remarkable specific capacitance of 3409.1 F/g at a high current density of 4.5 A/g is achieved when tested in 0.3M KI in 1M H₂SO₄ redox additive electrolyte (RE) compared to aqueous electrolyte (AE). Furthermore, we demonstrate the practical utility of RE by assembling a symmetrical supercapacitor, yielding an unprecedented energy density of 47.2 Wh/kg at a superior power density of 2.8 kW/kg. The device exhibits excellent cyclic stability (93.8%) and columbic efficiency (98.4%) after 10,000 continuous charge-discharge cycles, confirming the efficacy of potassium iodide-based redox additive electrolytes in conjunction with core-shell MOF electrodes for superior supercapacitor performance.



P26. Development of Green Carbon Dots and Metal Frameworks based nanocomposites for Printable Biosensors

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A biosensor functions by producing readable signals that directly correlate with the concentration of a target. Thus, have wide-ranging applications including disease monitoring (e.g., for COVID-19), drug development, and the detection of contaminants and pathogens. Electrochemical biosensors, in particular, are predominant in the market, constituting 80% of the industry, owing to their extensive use in healthcare and environmental monitoring. By integrating these sensing technologies with nanomaterials with high surface-to-volume ratios, and robust conductivities, challenges related to sensitivity, repeatability, and selectivity can be effectively overcome. We have produced the carbon dots (CDs) from biowaste such as bamboo leaves, citrus peels, imbued with unique functionalities and covalent bonds to form porous and adaptable host structures known as Metal-Organic Frameworks (MOFs). We propose hybrid structures combining bio-waste-derived CDs (BWCDs) and MOFs as an ideal foundation to develop a detection platform for TNF- α , a vital pro-inflammatory cytokine crucial for the early diagnosis of diseases such as Alzheimer's disease, sepsis, and cancer. The obtained nanomaterial allows the spatial distribution of BWCDs within MOF crystals, to facilitate antibody immobilization. Characterization of the material is achieved through effective techniques such as scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), and X-ray diffraction (XRD). Moreover, we will also explore an innovative technique known as scanning electrochemical microscopy by employing this material as an ink for printable biosensors, enabling the detection of minute concentrations of TNF- α through the study of electrochemical reactions at a micro-scale level.

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P27. Comparison of local surface properties of copper and mild steel under corrosion

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Corrosion is defined as the destruction of metal due to reaction with its environment. This process depends on many factors: composition, temperature, surface condition, dislocations, and many other metallurgical factors such as grain size, texture, chemical heterogeneity, phase transformation and residual stress. During the operation of metal structures, many different types of defects occur that affect the properties of the materials. Mechanical deformations and mechanical stability are most important for metals. So, for the successful use of these materials, it is necessary to know how these mechanical deformations (local dents, defects, scratches) affect their physical properties. These defects have local nature and for investigation effect of these defects need to use local methods too. AFM (atomic force microscopy), nanoindentation, micro-scratching techniques have been successfully used to investigate the physical properties of materials at the nanoscale levels.

In this work we investigated local properties during corrosion in distilled water of mild steel copper by AFM methods after local mechanical deformation (nanoindentation, micro-scratching, polishing). By kelvin probe force microscopy (KFM) surface potential after deformation changed on -300 mV in deformed area with additional modulation of surface potential correspond to local surface shape (bending). Some correlations during corrosion and mechanical deformation of mild steel magnetic domain distribution, surface potential, local friction properties were found by magnetic force microscopy (MFM) and friction force microscopy (FFM). Local surface morphology and roughness of copper and mild steel during corrosion were investigated.

This work was developed in the scope of the Project “Agenda ILLIANCE” [C644919832-00000035 | Project no. 46], financed by PRR – Recovery and Resilience Plan under the Next Generation EU from the European Union. This work also was supported, in terms of TEMA Research Infrastructure equipment, by the projects UIDB/00481/2020 and UIDP/00481/2020 - Fundação para a Ciência e a Tecnologia; and CENTRO-01-0145-FEDER-022083 - Centro Portugal Regional Operational Programme (Centro2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund.



P28. Polymeric Nanoparticles for Drug Delivery, using Bovine Serum Albumin for Prostate Cancer Treatment: An *In Vitro* Study

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Prostate cancer (PCa) is the second most prevalent type of cancer in the male population worldwide.^[1] The current treatments have many limitations, such as low specificity and drug resistance, which have serious consequences for the body. Researchers have focused on the development of advanced drug delivery systems to address these challenges. Polymeric nanoparticles (NPs) have been proposed as valuable drug delivery systems, with promising in vitro results in cancer cell lines. Bovine serum albumin (BSA) NPs represent a promising and eco-friendly approach for targeted drug delivery, with reported biocompatibility, stability, and biodegradability.^[2] The primary aim of this study was to synthesize bovine serum albumin (BSA) NPs using a genipin (GNP)-based cross-linking method to act as a carrier for cancer treatment, the antidepressant sertraline (STR), which has demonstrated potential efficacy in prostate cancer treatment. BSA NPs were synthesized using an emulsion method and characterized using Dynamic Light Scattering (DLS). After selecting the most appropriate synthesis method, the procedure for STR encapsulation was tested. The NPs were characterized by DLS, and the encapsulation efficiency was assessed using HPLC. The PNT-2 (normal prostate cells) and 22Rv1 (prostate cancer cells) cell lines were used in in vitro assays to evaluate their potential efficacy. These cell lines were exposed to BSA NPs with and without STR and their cytotoxicity was assessed. BSA NPs were successfully synthesized, presenting a hydrodynamic size distribution (200–400 nm) and polydispersity index of 0.183. STR was effectively encapsulated (82% efficiency) in the BSA NPs, which maintained good stability and monodispersity despite the formation of some aggregates. Exposure to BSA NPs slightly decreased the viability of PNT-2 and 22Rv1 cells, with no GNP toxicity. BSA NPs loaded with STR demonstrated the ability to affect cell viability. This study showed that BSA NPs have good encapsulation efficiency and act as effective STR carriers. BSA NPs loaded with STR caused a slight reduction in cell viability, which increased over time. This is a promising approach for treating prostate cancer due to the lower toxicity of BSA NPs loaded with STR compared to direct STR exposure. Further studies should extend the exposure time to assess the effects of BSA NPs loaded with STR and study their release mechanisms.



Acknowledgment

This work was developed within the project NanoPlanet (DOI 10.54499/2022.02340.PTDC), the project CICECO – Aveiro Institute of Materials, UIDB/50011/2020, UIDP/50011/2020 (DOI 10.54499/UIDP/50011/2020), and LA/P/0006/2020 (DOI 10.54499/LA/P/0006/20209), and the CESAM, UIDP/50017/2020, UIDB/50017/2020, LA/P/0094/2020, financed by national funds through FCT/the MCTES.

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P29. Sensitizing effect of Yb^{3+} ions on 1.53 μm broadband and 548nm upconversion green emissions of Er^{3+} -doped $\text{TeO}_2\text{--WO}_3\text{--GeO}_2$ glasses

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The Er^{3+} -doped transparent glasses were the significant materials to design solid state visible lasers, near infrared lasers, upconverters, sensors and fiber amplifiers. The effect of Yb^{3+} sensitization on 1.53 μm broadband and 548 nm upconversion green emissions in $\text{TeO}_2\text{--WO}_3\text{--GeO}_2\text{--ErF}_3\text{--YbF}_3$ (TWGERYb) glasses were studied. They were characterized through structural, optical absorption, near infrared and upconversion studies. The Judd-Ofelt theory was adopted to estimate several spectroscopic and radiative parameters. The laser characteristic parameters such as stimulated emission cross sections, gain band widths, figure of merit and quantum efficiencies were evaluated. Conveying the energy from Yb^{3+} to Er^{3+} ions and the reasons for non-radiative losses were highlighted. The quenching in luminescence of 1.53 μm broadband, the 548 nm upconversion green emissions and the enhanced decay time values due to self-absorption were studied. The fitting of decay curves of Er^{3+} : $^4\text{I}_{13/2}$ and Er^{3+} : $^4\text{S}_{3/2}$ emission states at higher Yb^{3+} concentrations (≥ 1.5 mol%) to Inokuti-Hirayama model were discussed. The TWGERYbx glasses containing $0.5\text{Er}^{3+}/2.5\text{Yb}^{3+}$ show proficiency to design 548 nm green solid-state lasers and 1.53 μm broadband fiber lasers.

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P30. Experimental study of electron beam welding parameters for joining copper pipes in heat pumps

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The demand for heat pumps is increasing around the world due to their energy efficiency and eco-friendly advantage, which calls for technological upgrading in manufacturing. Traditional brazing methods used during the assembly of heat pumps face a challenge of low production efficiency, high energy consumption, and environmental harm [1]. Given these challenges, improvements in manufacturing processes are crucial for achieving environmental sustainability. One potential solution is electron beam welding (EBW), which offers better control over heat input and reduces microstructural defects [2]. The parameters in the EBW process of joining copper pipes in heat pump systems are optimised to improve the quality and reliability of the weld.

Several experiments were carried out to investigate the behaviour of some EBW parameters in copper-copper joints. Two different sets of samples were examined, including sample 1 with a lower beam current and welding speed, and sample 2 with a higher beam current and welding speed. This meant that Specimen 1 registered a better heat distribution and full welds, while Specimen 2 showed a poor distribution and many imperfections. However, both samples showed satisfactory microstructures in the impact zone, ensuring uniform heat distribution.

The main findings support the fact that it is critical to optimise the beam current in combination with the welding speed to obtain good quality of the welds. The decrease in beam current and welding speed led to a significant improvement in the quality of the welds; better heat distribution was allowed, and defects were avoided. This means that with strict control of the parameters of the EBW, it should allow for much more reliable and efficient manufacturing when producing heat pumps. Our research will help develop welding technologies further. The microstructure features and mechanical properties of the EBW joints provided by our study are good reference points for the adoption of EBW in the heat pump industry. EBW will significantly enhance the production efficiency and sustainability in the production of heat pumps with better quality welds.

The present study was developed in the scope of the Project “Agenda ILLIANCE” [C644919832-00000035 | Project nº 46], financed by PRR – Plano de Recuperação e Resiliência under the Next Generation EU from the European Union, and had laboratory support from the Centre for Mechanical Technology and Automation (TEMA), projects UIDB/00481/2020 and UIDP/00481/2020.

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2nd Workshop on New Challenges of Bionanomaterials: Science, Technology, Application

The background of the slide is a solid blue color. In the four corners, there are decorative fractal patterns. These patterns are composed of many small, branching, and self-similar structures, resembling a combination of natural forms like coral or seaweed and mathematical fractals. The colors of these patterns are primarily yellow and orange, with some green and blue accents, creating a vibrant contrast against the blue background.

2nd Workshop on New Challenges of Bionanomaterials: Science, Technology, Application

**University of Aveiro
Portugal**

9 July, 2024



Modern state of Earth civilization show tendency with increase role of quality of people life. This is including, on the first-place, level of medicine, so, biology. In present days development of biomaterials, nano science and information technology give optimistic perspectives on this way direction and this allows more and more new horizons in Life sciences, Ecology, Green technologies, Education, Social organization society, etc. Thus, great opportunities open for young researchers in the realization they noble desires in understanding very difficult and very interesting fundamental laws of nature and to make practically a harmonious human future. Focusing, understanding and international exchange of knowledge are the basis for solving new questions in these areas. With this objective, we organize Workshop on Modern Problems of Bionanomaterials: Science, Technology, Application (WNCBM2024) with presentations and discussions specialists in Biomaterials, Nano science and Nano technology.

2nd Workshop New Challenges of Bionanomaterials: Science, Technology, Application, University of Aveiro, Portugal, 9 July, 2024

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Nanoassemblies / Surfaces
Modelling of Bionanomaterials
Bio-Inspired nanomaterials
Bio-nano measurement and microscopy
Nanobioanalysis in vitro
Nanotoxicology
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2nd Workshop on New Challenges of Bionanomaterials: Science, Technology, Application University of Aveiro, Portugal, 9 July, 2024	
9:00–9:10	WELCOME ADDRESS Dr. Gil Gonçalves Dr. Igor Bdikin
9:10–9:40	CHAIR: Dr. Gil Gonçalves and Dr. Igor Bdikin W3-O1. Addressing the ecotoxicity of micro(nano)plastics of polyhydroxybutyrate (biobased) and polymethylmethacrylate (petroleum-based) on <i>Danio rerio</i> physiology and behaviour Cátia Venâncio <i>Centre for Environmental and Marine Studies, Department of Biology, University of Aveiro, 3810-193 Aveiro, Portugal</i>
9:40 – 9:55	W3-O2. Protein-based nanomaterials as magnetic resonance imaging contrast agents Gabriela Guedes <i>Center for Cooperative Research in Biomaterials (CIC biomaGUNE), Basque Research and Technology Alliance, Parque Tecnológico de San Sebastian Paseo Miramón 194, 20014 Donostia-San Sebastian, Spain</i>
9:55 -10:10	W3-O3. Development of biobased polyesters derived from 2,5-furandicarboxylic acid and their sustainable nanostructures Lorenzo Ceparano <i>CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal</i>
10:10 – 10:25	W3-O4. A case study comparing the impacts of nanometric particles made of petroleum and biopolymers on freshwater organisms Miguel Oliveira <i>Centre for Environmental and Marine Studies, Department of Biology, University of Aveiro, 3810-193 Aveiro, Portugal</i>



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W1-O1. Addressing the ecotoxicity of micro(nano)plastics of polyhydroxybutyrate (biobased) and polymethylmethacrylate (petroleum-based) on *Danio rerio* physiology and behaviour

Miguel Oliveira¹, Carolina Frazão¹, Ricardo J. B. Pinto², **Cátia Venâncio^{1*}**

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- **Introduction and Objective:** The use of bioplastics to replace conventional plastics (petroleum-based) should be supported by ecotoxicological tests to assess potential impacts for ecosystems. Furthermore, this assessment should not only include standardized parameters, but should also begin to integrate behavioral traits that may be translated into potential effects on human health. This work aimed to evaluate the effects of the exposure to micro(nano)plastics (0.1, 1, 10, 100, and 1000 µg/L) of polyhydroxybutyrate (PHB-MNPLs) and polymethylmethacrylate micro(nano)plastics (PMMA-MNPLs) in the embryonic-larvae stage of *Danio rerio*.

- **Method:** The OECD 236 Fish Embryo Toxicity (FET) (2013) ¹ was adapted for a period of 120h, with monitoring of the following endpoints: mortality, malformations, heartbeats (only at 48h), hatching rate (from 48h onwards), and total length (at 120h). At the end of the 120h swimming-related parameters (total time active, total distance swam, thigmotaxis, and trajectory angles) were also evaluated.

- **Results:** PHB-MNPLs and PMMA-MNPLs exposure had no impact on mortality, malformations, or hatching rates of *D. rerio*. PMMA-MNPLs induced tachycardia at 100 and 1000 µg/L and reductions in larvae length at concentrations between 0.1 and 100 µg/L. The PHB-MNPLs were able to induce effects in fish swimming-related parameters, similar to those induced by PMMA-MNPLs (decreased total time active under light periods; or a decrease in high amplitude movements at 0.1-10 µg PHB-MNPLs/L, and 100 and 1000 µg PMMA-MNPLs/L also under light periods).

- **Discussion/Conclusion:** This study highlighted the need to study and compare the potential toxicity of biobased or fuel-based polymers.

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W1-O2. Protein-based nanomaterials as magnetic resonance imaging contrast agents

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Magnetic resonance imaging (MRI) has revolutionized medical diagnostics by offering non-invasive, high-resolution imaging without radiation exposure. While MRI provides exceptional anatomical and molecular detail, it often requires gadolinium-based contrast agents to enhance diagnosis sensitivity and specificity. However, recent concerns about gadolinium toxicity have prompted a search for alternative agents with better stability and effectiveness. Additionally, the lack of specificity in current contrast agents underscores the need for a shift towards targeted contrast agents, which could significantly improve disease detection and treatment monitoring, ultimately enabling personalized medical interventions.[1]

Drawing inspiration from Nature, protein-stabilized nanomaterials offer the opportunity to design bioinspired high-quality nanomaterials that combine unique physicochemical properties with the biocompatibility, stability, and water solubility of proteins. Additionally, using proteins to template the synthesis of nanomaterials provides environmentally friendly and straightforward protocols. Consensus tetratricopeptide repeat (CTPR) proteins are designed proteins that are particularly notable for their robustness and mutational permissibility, allowing the introduction of metal coordination sites without a substantial impact on the protein structure.[2] The use of CTPR designed proteins enables better control of the nanomaterials' properties, and offers a fully customizable platform for the introduction of specific functional motifs.[3-4]

For instance, histidine-based metal-binding sites were introduced into CTPR proteins for the stabilization of iron oxide nanoparticles (Prot-IONPs) with tailored relaxivity properties, which enabled their exploration as MRI contrast agents. [5] Moreover, two different strategies were explored to target the Prot-IONPs to specific pathologies. In a first approach, the protein scaffold in Prot-IONPs was modified with alendronate to target calcifications in atherosclerotic plaques. In a second approach, the protein scaffold was engineered to display different binding peptides with high affinity towards KEAP1 and tankyrase, relevant potential therapeutic targets in neurodegenerative diseases and cancer.

In conclusion, this study serves as a proof-of-concept for the versatility and potential of the Prot-NPs in biomedical applications through the development of MRI contrast agents with targeting ability. Moreover, we showcase designed proteins as a platform that allows the scaffolding of diverse nanomaterials that can be finely tuned to target and treat different conditions either by simply changing the protein sequence or by straightforward post-synthetic modifications.

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W1-O3. Development of biobased polyesters derived from 2,5-furandicarboxylic acid and their sustainable nanostructures

Lorenzo Ceparano^{*}, Luísa Figueiredo, Beatriz Agostinho, Vinícius de Paula,

Sónia A. O. Santos, Ricardo J.B. Pinto, Andreia F. Sousa

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Nowadays, the massive use of polymers has been increasing, with the vast majority deriving from fossil resources. Therefore, the quest for potentially more sustainable alternatives has increased, with polymers of renewable origin emerging as promising options. New biobased polymers using renewable-based monomers, such as FDCA and derivatives with different diols from renewable origin, stand out as a perfect example, boasting interesting mechanical, thermal, and barrier properties [1][2], with promising applications, particularly as fibers for textiles or in the packaging sector. The development of nanostructured systems of these polymers could expand their range of applications even further, including in highly specialised sectors such as medicine.

This work aims precisely to evaluate the preparation of nanoparticles (NPs) of poly(ethylene 2,5-furanodicarboxylate), known as PEF, and poly(diethylene 2,5-furanodicarboxylate), known as PDEF, through the nanoprecipitation method. The impact of various experimental parameters was assessed, including agitation methodology, choice of antisolvent and surfactants, the volume ratio of the polymeric solution and the aqueous phase, as well as the precursor's concentration and chemical structure. The influence of these variables on the size, morphology, and surface charge of the nanostructures was examined using electron microscopy, dynamic light scattering, and zeta potential analysis, aiming to establish reliable and scalable methodologies in order to control the size of NPs according to the applications they are needed.

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2nd Workshop on New Challenges of Bionanomaterials: Science, Technology, Application
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W1-O4. A case study comparing the impacts of nanometric particles made of petroleum and biopolymers on freshwater organisms

Cátia Venâncio¹; Miguel Tamayo-Belda²; Isabel Lopes¹; Ricardo J. B. Pinto³; Francisca Fernandez-Piñas²; Roberto Rosal⁴; **Miguel Oliveira^{1*}**

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- **Introduction and Objective:** The European Union Directive on single-use plastics has prompted and encouraged the development and adoption of more sustainable materials, such as bioplastics. However, to define bioplastics as a more environmentally friendly option comparisons must be performed with fossil-fuel based plastics. Considering the scarce ecotoxicological profile of polymers (based mostly on lower trophic levels), this work aimed at evaluating the toxicity of a biopolymer [Polylactic Acid (PLA)] and three fossil-based polymers [Low density polyethylene (LDPE), Polypropylene (PP), and Polystyrene (PS)] on two secondary consumers (*Hydra viridissima* and *Danio rerio*), at concentrations of 0.001, 0.01, 0.1, 1, and 10 mg/L.

- **Methods:** Mortality and malformation (Trottier et al., 1997)¹ and regeneration and feeding (Trottier et al., 1997)¹ assays were carried out with *H. viridissima* exposed for 96h, while the OECD 236 Fish Embryo Toxicity (FET) (2013)² adapted to 120h was carried out with *D. rerio*. Polymers' suspensions characterization included FTIR spectra, ζ -potential, and DLS.

- **Results:** The PP and LDPE were the most toxic polymers to *H. viridissima* morphology, while the PLA was the polymer inducing the highest effect on post-exposure feeding rates and promoted faster regeneration rates. In *D. rerio*, the PLA and PP induced significant changes, at similar magnitude, in fish swim trajectory turning frequency (between 35-80% reduction relatively to the control), as well as in swimming distance (decrease of around 40% relatively to the control) at the three highest tested concentrations. All polymer suspensions have shown a tendency for aggregation over time.

- **Discussion/Conclusion:** The selected endpoints were sensitive, indicating the ability of biopolymers to induce ecotoxicity in the same order of magnitude as petroleum-based ones. There is a need to provide ecotoxicity data comparing bio- and petroleum-based polymers for informed decision-making.

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Workshop on “ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES” (9 July 2024)





Workshop on Workshop on “ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES” (9 July, 2024)



The Workshop on Advanced Materials: Applications and Technologies (AMAT 2024) aims to bring together researchers, academics, industrial professionals, and students to participate in the discussion on advanced materials. This event will feature talks from leading scientists/academics in the field. We look forward to seeing you there!

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Workshop on “ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES” (9 July 2024)	
10:45–10:55	WELCOME ADDRESS Dr. Indrani Coondoo Prof. Georgina Miranda
10:55–11:30	CHAIR: Dr. Indrani Coondoo Keynote talk Functionalized nanofibers by electrospinning For Energy applications Prof. Bernardo Almeida University of Minho, Portugal
11:30–12:15	Plenary Lecture 3D Printed Porous Ceria Ceramics for Solar Thermochemical Production of Sustainable Fuels Prof. Robert Pullar Università Ca' Foscari Venezia, Italy
12:15–14:00	Lunch
14:00–14:30	Keynote talk One-dimensional charge transporting columnar mesogens for optoelectronic applications Dr. Dharmendra Pratap Singh Université du Littoral Côte d'Opale (ULCO), France



Workshop on “ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES”
University of Aveiro, Portugal, 9 July, 2024

Plenary Lecture

3D Printed Porous Ceria Ceramics for Solar Thermochemical Production of Sustainable Fuels

Robert C. Pullar

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Ceria can reduce to nonstoichiometric $\text{CeO}_{2-\delta}$, undergoing partial and reversible reduction at elevated temperatures, making it an ideal material for the solar thermochemical fuel production (STFP) of renewable fuels from the splitting of water to produce H_2 , or splitting CO_2 to CO for the production of synthetic sustainable fuels. Ceria has the required redox capabilities, is thermally stable and resistant to sintering during thermochemical cycling over the typical 900-1500 °C temperature range used, has an unusually high entropy change associated with oxygen exchange resulting in lowered temperature swings between the reduction and oxidation steps compared to other non-stoichiometric redox materials, and has rapid reaction kinetics and oxygen diffusion rates. Macroporous robocast (additive manufacturing / 3D printed) ceria structures in the form of “woodpile” type scaffolds should be ideal for such applications. In this presentation we will look at the development of such materials.



Workshop on “ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES”
University of Aveiro, Portugal, 9 July, 2024

Keynote talk

W2-I1. Functionalized Nanofibers by Electrospinning for Energy Applications

D. Santos^{1,2}, A. Handa¹, R. Baptista¹, E. Gomes¹, T. Rodrigues¹, **B.G. Almeida¹**

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Peptides consist of sequences of amino acids that can self-assemble into various supramolecular structures, such as nanospheres, nanotubes, and nanowires, exhibiting quantum confinement and photoluminescence [1-5]. In this respect, non-centrosymmetric chiral dipeptide-based nanomaterials, are a promising class of compounds for applications in environmentally friendly optoelectronic devices and for energy harvesting, thanks to their biocompatibility, ease of fabrication, and functionalization [1].

Hybrid composite bionanomaterials produced by electrospinning present the possibility of functionalizing polymeric nanofibres with active organic molecules, depending on the physical and chemical properties of these chiral dipeptides [2-5]. These materials have many advantages, such as excellent thermal and mechanical stability, high piezoelectricity, and excellent optical properties. Thus, here we report the fabrication and characterization of hybrid systems based on the chiral cyclo-dipeptides L-Tryptophan-L-Tryptophan and cyclo-L-Tryptophan-L-Tyrosine incorporated into biopolymer electrospun fibers [2,3], and the production and analysis of hybrid micro/nanofibers of the linear dipeptide Boc-L-phenylalanyl-L-Leucine and Boc-L-phenylalanyl-L-Isoleucine [4,5].

The structural, morphological, mechanical and optical properties of the hybrid composites were measured showing an enhancement as compared to the bulk counterparts. Remarkably, the composite micro/nanofibers displayed semiconducting dielectric characteristics with bandgap energies ranging from 4 to 5 eV [4,5]. The dielectric properties of the fibers were analyzed using impedance spectroscopy, considering temperature and frequency variations. The successful integration of the dipeptide was confirmed through Maxwell–Wagner interfacial polarization, while the permittivity contributions were studied based on the Havriliak–Negami model [4,5].

In addition, the fibers exhibited efficient pyroelectric and piezoelectric responses. As an example, a piezoelectric nanogenerator capable of producing $0.18 \mu\text{Wcm}^{-2}$ of power density and have a piezoelectric coefficient of 57 pC/N demonstrated for Cyclo (L-Trp-L-Trp)@PLLA [2].

Beyond purely organic composites, these hybrid structures can be further combined with magnetic inclusions giving additional degrees in device design. In this respect



magnetoelectric responses are achieved and flexible magnetocaloric fibers can be built for magnetic refrigeration [6].

Thus, the results highlight the impact of dipeptide nanostructures and magnetic inclusions on dielectric, magnetoelectric, pyroelectric and piezoelectric properties, indicating that these hybrid systems are very promising for applications in the field of environmentally friendly and biocompatible nanoenergy harvesting, magnetic refrigeration and piezoelectric generators for portable and wearable devices.

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Workshop on “ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES”
University of Aveiro, Portugal, 9 July, 2024

Keynote talk

W2-I2. The one-dimensional Charge Transporting Columnar Mesogens for Optoelectronic Applications

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Recently, columnar mesogens have emerged as Hole transport materials (HTMs) rendering a significant impact on the effectiveness of organic electronic devices [1,2]. The columnar mesogens exhibit hexagonal (Col_h) or rectangular (Col_r) columnar phases offering an impressive 1D hole mobility in the order of 0.1 to 10⁻⁴ cm²V⁻¹s⁻¹ which is found to be dexterous than most existing polymeric hole transport materials [2]. The charge transport mechanism in these mesogens is mainly governed by the hopping process in which electrons/holes unidirectionally migrate from one π -conjugated core to another [3]. This presentation describes the role of liquid crystalline columnar materials as HTL and their impact on the performance of optoelectronic devices.

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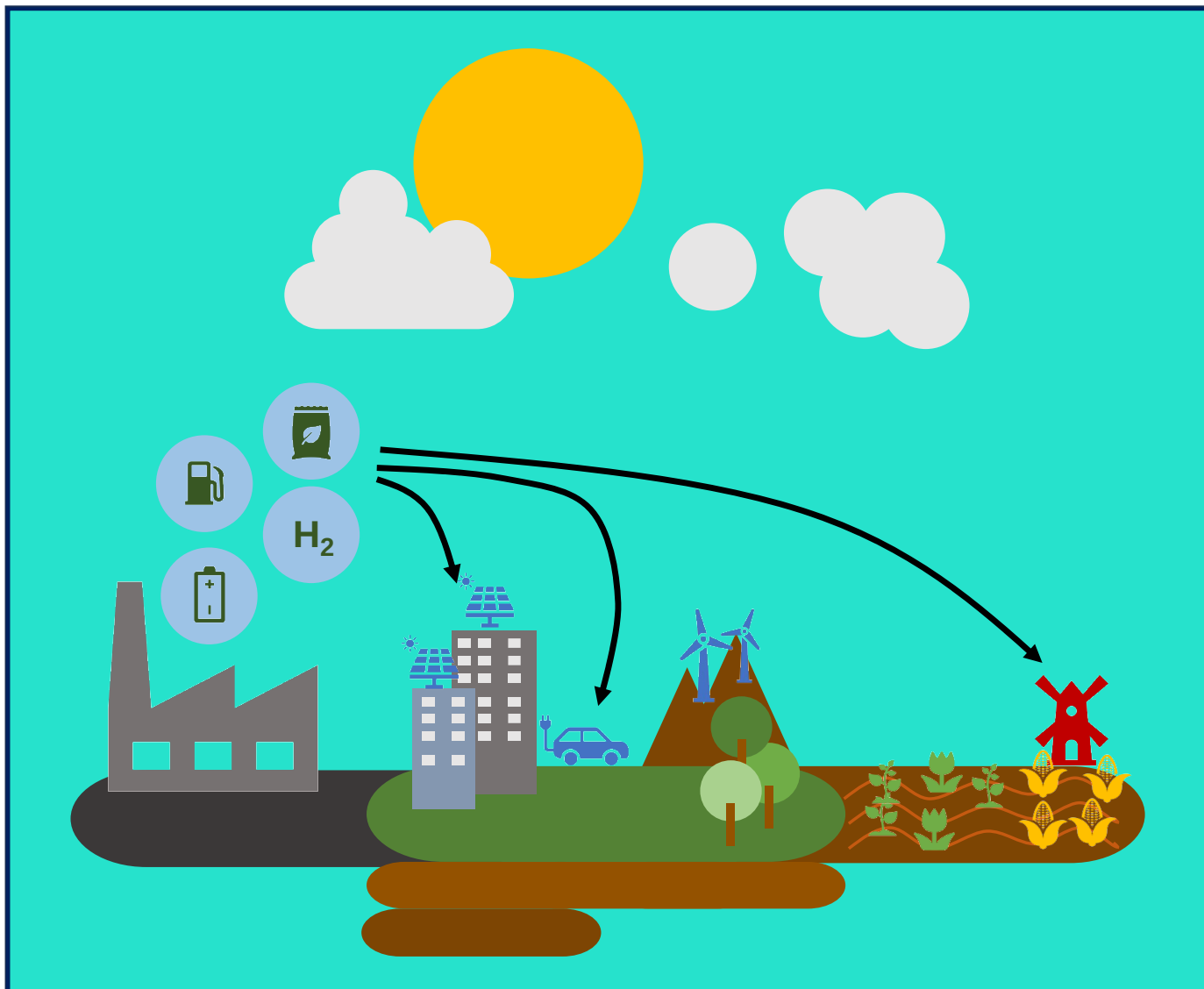
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2nd International Workshop on “Modern Trends in Energy Research”,

University of Aveiro, Portugal, July 9, 2024
(IWMTER-2024)





2nd International Workshop on “Modern Trends in Energy Research” 9 July 2024, Aveiro, Portugal

Topics:

Green Hydrogen: Production, Storage & Transport
Fuel Cells/Electrolysers
Electrochemical Synthesis of Fuels and Chemicals
Batteries & Supercapacitors
Nanocatalysis & Electrocatalysts

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2nd International Workshop on “Modern Trends in Energy Research”, University of Aveiro, Portugal, July 9, 2024 (IWMTER-2024) Affiliation of workshop speakers: Centre for Mechanical Technology and Automation – TEMA, Department of Mechanical Engineering, University of Aveiro, Portugal Session Chairs: Duncan Paul Fagg / Laura Holz	
14:30–15:00	WELCOME ADDRESS and workshop introduction D. Pukazhselvan
	Planary Lecture: Highlights to the advanced anode active materials for rechargeable batteries D. Pukazhselvan
15.00–15.20	Invited Talk-1: Electrospun $[\text{Ca}_2\text{CoO}_{3-\delta}]_{0.62}[\text{CoO}_2]$ nanofibres: Improving the oxygen reaction kinetics in solid oxide fuel cell cathodes Allan J. M. Araújo
15.20–15.35	Invited Talk-2: Synthesis of novel electrolytes for proton ceramic membrane Reactors Alfredo S. B. Luemba
15.35–15.50	Invited Talk-3: Low-Cost $\text{Ca}_2\text{Fe}_2\text{O}_5$ Catalysts Synthesized by Reactive Firing of Calcite and Siderite for Application in Alternative Energy Technologies Isabel Antunes
15.50–16.10	Coffee break / Open discussions
16:10–16:30	Planary Lecture: Thermogravimetry: how to build a kinetic model. A case study of the oxidation of niobium nitride Vanessa Graça
16:30–16:45	Invited Talk-4: Life cycle assessment of energy-dense fuels from electrochemical biogas conversion J.K. Ravindran
16:45–17:00	Invited Talk-5: Harnessing Energy from Salinity Gradients through Reversible Electrodialysis Eduardo Durana
17.00–17.20	Invited Talk-6 / Key note address and closing remarks Proton conductivity in doped barium cerate under nominally dry conditions Francisco JA Loureiro



2nd International Workshop on “Modern Trends in Energy Research”
University of Aveiro, Portugal, 9 July, 2024

Plenary Lecture

Highlights to the advanced anode active materials for rechargeable batteries

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Abstract: Rechargeable batteries play an important role in our daily lives as they are required for our day-to-day activities, for example in portable electronic gadgets, household appliances, vehicles, etc. Over time, several rechargeable battery systems have been developed, where sodium and lithium ion batteries emerge particularly noteworthy due to their impressive energy density and commercial success. One area of intense R&D focus in the literature is the development of new materials for the anode side of rechargeable batteries [1, 2]. Anode active materials can be categorized into three main types: intercalation type materials (e.g., natural graphite), conversion type materials (e.g., Fe₂O₃), and alloying type materials (e.g., Si). A popular intercalation material, natural graphite, is a widely used active anode material (theoretical capacity of 372 mAh/g) in commercial Li ion batteries (the experimentally observed capacity is typically between 200-300 mAh/g). This value can be considered as a reference capacity and research efforts are made worldwide to invent materials with higher capacity than that of natural graphite. Breakthrough material tailoring strategies were reported in the literature, and it is possible to develop materials with capacity several times higher than that of natural graphite, for example, geometry tailored silicon can reach capacity as high as 3000 mAh/g [3]. Thus far, in a broader context, intercalation materials have been the most successful for metal ion batteries, but ongoing efforts aim to tailor cycle sustainable conversion-type and alloying-type anode active materials. In our laboratory, we are studying various intercalation materials including metal organic frameworks (MOF), pillared/doped reduced graphene oxide, and pyrolyzed MOF structures. Our research indicates that a potential capacity range of 400-700 mAh/g for hundreds of cycles is possible to achieve through intercalation type materials.

Keywords: Rechargeable batteries, Anode active materials, electrochemistry, ionic intercalation.

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*2nd International Workshop on “Modern Trends in Energy Research”
University of Aveiro, Portugal, 9 July, 2024*

Plenary Lecture

Thermogravimetry: how to build a kinetic model. A case study of the oxidation of niobium nitride

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Abstract:

Thermogravimetric analysis (TGA) is a powerful technique for studying the changes in physical and chemical properties of materials by measuring the mass change as function of temperature (with constant heating rate) or as function of time (with constant temperature and/or constant mass loss) [1]. However, TGA method can also be used to study the kinetics of chemical reactions [2]. Hence, the current work aims to address the basic theory of reaction kinetics complemented with a detailed analysis on the thermal oxidation of niobium oxynitride (NbN_xO_y) as a case study. In this regard, the oxidation of NbN_xO_y was kinetically modeled using the TGA data and Kinetics Neo software from Netzsch. It was found that the experimental data of thermal oxidation of NbN_xO_y can be fitted by employing a model that comprehend two single steps ($A \rightarrow B \rightarrow C$) [3]. The first was assigned to an Fn-type reaction whereas the second was ascribed to the Avrami model reaction. The latter justified by the identification of an amorphous-to-crystalline phase transformation during thermal oxidation.

Finally, by establishing a kinetic model it is possible, for example, to predict the degree of conversion for a given temperature condition, which in our case study allows to predict the time necessary for the complete oxidation of niobium oxynitride samples with different O/N ratios.

In conclusion, kinetic analysis can give deep insight into detailed chemical mechanism been a valuable tool to understand and optimize materials.

Keywords: thermogravimetry, kinetic model, kinetic parameters, niobium oxynitride

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2nd International Workshop on “Modern Trends in Energy Research”
University of Aveiro, Portugal, 9 July, 2024

Keynote talk

W3-I1. Electrospun $[\text{Ca}_2\text{CoO}_{3-\delta}]_{0.62}[\text{CoO}_2]$ nanofibres: Improving the oxygen reaction kinetics in solid oxide fuel cell cathodes

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Abstract: Recent advancements in Solid Oxide Fuel Cells (SOFCs) highlight that the commercialization of this technology is significantly hindered by the slower kinetics of the oxygen reduction reaction (ORR) of cathode materials.¹ The misfit calcium cobalt oxide $[\text{Ca}_2\text{CoO}_{3-\delta}]_{0.62}[\text{CoO}_2]$ (CCO) demonstrates potential in this area due to its rapid surface-exchange kinetics and a thermal expansion coefficient well-matched with standard electrolytes.^{2,3} However, its performance is compromised by the poor bulk oxygen ion conduction,³ which restricts oxygen diffusion to the surface pathway, where microstructure is crucial. This study investigates an alternative method for synthesizing CCO materials using electrospinning (ES), creating a morphology composed of small, platelet-like grains with increased surface area and a higher aspect ratio when compared to powders produced by the state-of-the-art solid-state reaction (SSR) route. The electrode films derived from the ES-based powders were found to exhibit a significantly improved electrochemical performance, where the total polarisation resistance is reduced by 60 % to 69 % within the temperature range of 800 °C to 600 °C, compared to the sample produced using the SSR-based powders. Additionally, single cell tests demonstrate an 8.4-fold increase in peak power density at 700 °C. Overall, our research underscores electrospinning as a promising alternative for producing CCO cathodes with enhanced electrochemical properties.

Keywords: SOFC cathode, misfit calcium cobaltite, electrospinning, microstructure.

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*2nd International Workshop on “Modern Trends in Energy Research”
University of Aveiro, Portugal, 9 July, 2024*

Keynote talk

W3-I2. Synthesis of novel electrolytes for proton ceramic membrane reactors

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Abstract

Global energy and climate change are among the world's main problems today, due to an extensive dependence on fossil fuels. In this context, the European Union (EU) has organized policies to foster the adoption of efficient and sustainable renewable energy sources, eclipsing the dominance of fossil fuels. This massive endeavor finds its foundation in the European Green Deal (EGD), a comprehensive framework designed to propel Europe towards carbon neutrality by 2050 while ensuring the provision of clean, affordable, and secure energy across the EU [1-2]. In line with the energy transition, biogas can play a very important role in this goal, as these gases can be used in the transformation of the global energy system in accordance with the International Energy Agency (IEA).

Following these aims, the current study proposes an electrochemical device to form green syngas (a mixture of CO and H₂) from a biogas precursor (CO₂ + CH₄), by a direct electrochemical process through a proton-conducting ceramic membrane. The focus of this research is related to the development of alternative electrolyte materials with improved chemical tolerance against biogas composition. In this regard, chalcogenide perovskite protonconducting ceramics made of BaZrS₃ (BZS) were prepared from the parent oxide BaZrO₃ phase using a mechanochemical activation route (under dry milling at 650 rpm for 7 h). Then, sulfurization was performed by exposing the BaZrO₃ powders to a carbon disulfide atmosphere, which was introduced through a bubbler filled with liquid CS₂ (99.9%, Sigma-Aldrich), using Ar as the carrier gas (5 mL min⁻¹). X-ray diffraction (XRD) measurements revealed pure phase formation. Stability measurements in CO₂ and CH₄ atmospheres revealed no chemical interreaction with the exposed atmosphere.

Keywords: Ceramic electrolyzer; biogas; syngas; electrolyte.

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*2nd International Workshop on “Modern Trends in Energy Research”
University of Aveiro, Portugal, 9 July, 2024*

Keynote talk

W3-I3. Low-Cost $\text{Ca}_2\text{Fe}_2\text{O}_5$ Catalyst Synthesized by Reactive Firing of Calcite and Siderite for Application in Alternative Energy Technologies

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Abstract:

In this work, one demonstrates the feasibility of processing the brownmillerite phase $\text{Ca}_2\text{Fe}_2\text{O}_5$ by reactive firing of calcite and natural siderite, for prospective catalytic applications ^[1]. Thermogravimetry and X-ray diffraction were used to monitor the decomposition of precursors and its dependence on heating rate and atmosphere. Taguchi planning allowed one to assess the impact of firing temperature, dwell time, and rate of heating on the conversion of precursors from X-ray diffraction data analysis. Additionally, the effect of the typical gangue components of the natural siderite precursor in the brownmillerite structure formed and in the onset of minor phases was studied. Firing in non-oxidizing atmospheres was found that may prevent the onset of CaFe_2O_4 secondary phase. Testing of processed $\text{Ca}_2\text{Fe}_2\text{O}_5$ as water gas shift catalysts showed a positive impact on conversion of CO and H_2 yield, compared to tests conducted without the catalyst ^[2].

Keywords: Siderite, Brownmillerite, Solid state synthesis, Water gas shift

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*2nd International Workshop on “Modern Trends in Energy Research”
University of Aveiro, Portugal, 9 July, 2024*

Keynote talk

W3-I4. Life cycle assessment of energy-dense fuels from electrochemical biogas conversion

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Abstract: As concern about climate change rises, the need for sustainable alternatives becomes imperative. Producing and using green, energy-dense fuels from biomass appears promising for decarbonization and the reduction of environmental damage from fossil fuels. This study explores the impacts associated with liquid green fuels made through the electrochemical conversion of biogas, aiming to bridge gaps in the literature and promote sustainable transport systems.

A review of biomass conversion technologies, such as anaerobic digestion followed by electrolysis and Fischer-Tropsch (FT) synthesis shows that, despite their potential to reduce greenhouse gas emissions, there exist some significant contradictions as to their sustainability. Okeke et al. [1] shows a significant reduction in environmental impacts while Navas-Anguita et al. [2] shows increased emissions. This study aims to resolve the aforementioned discrepancies and provide a comprehensive understanding of the environmental impacts associated with these fuels with the use of the life cycle assessment (LCA) methodology.

Results showed that, the production of 1 kg Fischer-Tropsch (FT) fuels from biomass led to a global warming potential of 1.99 kg CO₂ eq, terrestrial ecotoxicity of 9.49 kg 1.4-DCB eq and human carcinogenic toxicity of 4.44 kg 1.4-DCB eq. Electrolysis was the hotspot in the production process with the highest impact in all 6 categories analyzed, due to its large electricity demand. The comparison of the combustion of 1 kg FT-diesel to 1 kg fossil-based diesel showed that FT-diesel has significantly lower impacts in 4 out of 6 categories analyzed, while having a higher value for ionizing radiation.

By addressing the inconsistencies [3] existing in the literature and advocating for a standardized approach to LCAs of alternative fuels, this research aims to provide a better understanding of the production and use of these fuels as well as future research directions in LCAs of these fuels. The findings of this study are expected to be used by



policymakers and industry stakeholders to make informed decisions about the integration of these fuels into sustainable transport systems.

Keywords: Liquid green fuels, Life cycle assessment, Electrochemical biogas conversion

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2nd International Workshop on “Modern Trends in Energy Research”
University of Aveiro, Portugal, 9 July, 2024

Keynote talk

W3-I5. Reversible electrodialysis: a salinity gradient power source

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Abstract: Energy demand in the last decades has increased globally, mainly caused by population growth and rising living standards in emerging economies. Greenhouse gas emissions and global warming impacts are, therefore, compelling for alternative clean and sustainable energy resources [1]. Salinity Gradient Power (SGP) is a clean and renewable energy source with a global potential based on the salinity difference between sea and river water. Theoretically, it is possible to extract 0.8 kilowatts per cubic meter of fresh water, allowing a prediction of worldwide harness capacity of 980 GW from river water and 18 GW from wastewater running to the seas [1]. Reverse electrodialysis (RED) is a technology that harnesses the potential of SGP to produce electricity. This non-intermittent electrochemical process employs ion-exchange membranes (IEMs) for Donnan potential generation. The device's open circuit voltage (OCV) results from the voltage across each IEM stacked. The electrochemical potential at the electrodes is converted to electricity by a reversible redox reaction [2]. RED, when used with water effluent, can significantly increase the energy efficiency of industrial processes, demonstrating the practical benefits of this technology [3]. In this work, a RED device laboratorial setup was constructed, comprising a stack of 11 IEMs. The stack was fed with different salinity gradients (0.017 - 0.5 M NaCl), under different flow rates (1 - 14 mL min⁻¹). The results highlighted the pivotal roles of solution concentration and flow rate in determining the stack performance, with significant diffusion limitations notable under non-optimal conditions. This research, thus, provides insights into the peak operational parameters of the RED device, providing guidelines for other membrane processes focused on energy conversion based on SGP.

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Keywords: Salinity gradient energy, ion-exchange membrane, Donnan potential, Renewable energy.

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2nd International Workshop on “Modern Trends in Energy Research”
University of Aveiro, Portugal, 9 July, 2024

Keynote talk

W3-I6. Proton conductivity in doped barium cerate under nominally dry conditions

Francisco J. A. Loureiro^{1,2,*}, Domingo Pérez-Coll³, Vanessa C. D. Graça^{1,2}, Laura I. V. Holz^{1,2},
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Abstract: In addition to well-known potential applications, such as fuel cells, electrolyzers, and sensors, ceramic proton conductors have also been suggested for chemical synthesis, where hydrogenation or dehydrogenation reactions can be tailored electrochemically toward a desired chemical product [1]. Yttrium-doped barium cerate, BaCe_{1-x}Y_xO_{3-δ} (BCY), stands out as one of the most interesting materials at lower temperatures due to its superior proton conductivity under these conditions [2]. Nonetheless, BCY is commonly discarded due to its poor chemical stability towards hydroxide or carbonate formation [2]. The current work, therefore, combines impedance spectroscopy, thermogravimetric analysis, coulometric titration, and defect chemistry modeling to assess the limits for pure protonic conductivity in BaCe_{0.9}Y_{0.1}O_{3-δ} (BCY10) in nominally dry atmospheres ($p_{\text{H}_2\text{O}} \sim 10^{-4}$ to 10^{-5} atm, at low temperatures <600 °C). In this regard, for $T \geq 450$ -500 °C, where dehydration of the sample becomes significant, mixed conduction of both protons and oxygen ions is relevant. Nonetheless, below this temperature, the protonic conductivity of BaCe_{0.9}Y_{0.1}O_{3-δ} (BCY10) was determined to be 10^{-3} S cm⁻¹ at 350-400 °C, which is orders of magnitude higher than the oxide ionic and electronic conductivities. This remarkable performance allows for the applicability and stability of BCY10 to industrially relevant chemical synthesis reactions to be maintained, while still being hydrated. Interestingly, this peculiar characteristic of BCY10 is insufficiently highlighted in current literature, and yet it is a highly desirable property for a wide range of chemical de-hydrogenation/hydrogenation reactions where the presence of traditional levels of humidification (e.g., $p_{\text{H}_2\text{O}} = 10^{-2}$ atm) would otherwise lead to unwanted side reactions. For these reasons, it is expected that BCY10, and related doped barium cerates, can take a new role in the electrochemical promotion of chemical reactions in atmospheres of very low humidity, with a significant impact on the future of proton-ceramic conductors.

Keywords: SOFC cathode, misfit calcium cobaltite, electrospinning, microstructure.

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5th Workshop on Characterization and Analysis of Nanomaterials University of Aveiro, Portugal, July 9, 2024



Progress in science depends mainly on the level of experimental technology. Currently, interest in nanomaterials has led to many technological advances and has opened new horizons in understanding nature. Success in these ways possible by the development and standardization of methods for determining the characteristics of nanomaterials: X-ray diffraction, electron microscopy, atomic force microscopy, Raman spectroscopy, X-ray photoelectron spectroscopy, modeling of nanostructures, etc. A thorough knowledge of these methods is a necessary basis for work in modern science. The major aim of this workshop is to give a detailed description of principles and current state of the basic methods for characterization of nanomaterials.

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5th Workshop on Characterization and Analysis of Nanomaterials University of Aveiro, Portugal, July 9, 2024	
17:20-17:30	WELCOME ADDRESS Dr. Igor Bdikin, Dr. Gil Gonçalves
17:30-17:55	CHAIR: Dr. Igor Bdikin and Dr. Laura Holz <i>Keynote talk</i> W1-I1. X-ray diffraction (XRD) Dr. Laura Holz University of Aveiro, Aveiro, 3810-193, Portugal
17:55-18:30	<i>Plenary Lecture</i> X-ray Microtomography for materials characterization Prof. Dr. Isabel Duarte University of Aveiro, Aveiro, 3810-193, Portugal
18:30-19:00	W1-O1. Atomic force microscopy (AFM) Dr. Igor Bdikin University of Aveiro, Aveiro, 3810-193, Portugal
19:00-19:15	Close/discussions



5th Workshop on Characterization and Analysis of Nanomaterials
University of Aveiro, Portugal, 9 July, 2024

Plenary Lecture

X-ray Microtomography for materials characterization

Isabel Duarte *

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X-ray Microtomography (μ CT) has emerged as a powerful technique for non-destructive three-dimensional imaging and characterization of materials at micrometer to sub-micrometer resolutions. This plenary lecture provides a comprehensive overview of the principles, methodologies, and applications of X-ray Microtomography in materials science and engineering.

The lecture explores a wide range of applications [1-5], across various material classes including porous and cellular materials, and composites. Case studies (e.g. tissue engineering scaffolds, tooth structures and metal foams) demonstrate how X-ray Microtomography, coupled with 3D image processing, is utilized for analysis of internal structures, assessing parameters such as pore size and porosity.

Through this presentation, attendees gain insights into the capabilities and limitations of X-ray Microtomography as a versatile tool for understanding material properties, manufacturing processes, and structural integrity across various engineering domains.

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5th Workshop on Characterization and Analysis of Nanomaterials
University of Aveiro, Portugal, 9 July, 2024

Keynote talk

W4-I1. X-ray diffraction: A powerful technique for materials characterization

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One of the most important methods for determining a material's crystalline phases is X-ray diffraction. The method is non-destructive and retrieves information on a solid material's crystallographic structure using high-energy electromagnetic radiation (X-rays) with a wavelength on the order of the atomic spacings of crystals [1]. This lecture is intended for PhD candidates pursuing studies in materials science, chemistry and physics. This session covers the fundamental ideas of XRD, including the generation of X-rays, diffraction theory, the interpretation of diffraction patterns, the instrument, crystal structure determination, sample preparation and the advantages of a powder diffraction method.

This lecture seeks to give a thorough understanding of XRD's theoretical and practical applications. Participants will be able to apply XRD techniques to their research projects and contributing to the advancement of their respective fields.

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5th Workshop on Characterization and Analysis of Nanomaterials
University of Aveiro, Portugal, 9 July, 2024

W4-O1. Atomic force microscopy methods for materials characterization

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The ability to use organic microstructures opens huge prospects in electronics and medicine. But to effectively model and use them, research methods with the same resolution at the micro level are required. Atomic force microscopy (AFM) is one of such methods, which, in addition to high resolution, allows one to determine physical properties at the local level as well.

Organic materials, having a complex crystalline structure, often demonstrate the tendency and possibility of additional microscopic ordering with the formation of microstructures - films, rods, fibers, tubes, etc. The physical characteristics of such microstructures at the local level are highly dependent on the orientation and location of measurements. AFM methods allows to simultaneously obtain a real topographic image and an image of the distribution of a physical parameter, which is strictly correlated with the topography at each point of the image.

Here we show the piezoelectric properties of some organic materials (amino acids, ribonucleosides, P(VDF-TrFE, triglycine sulfate, diphenylalanine peptide) and the characteristics of these properties depending on their microstructure.

This work was developed in the scope of the Project “Agenda ILLIANCE” [C644919832-00000035 | Project no. 46], financed by PRR – Recovery and Resilience Plan under the Next Generation EU from the European Union. This work also was supported, in terms of TEMA Research Infrastructure equipment, by the projects UIDB/00481/2020 and UIDP/00481/2020 - Fundação para a Ciência e a Tecnologia; and CENTRO-01-0145-FEDER-022083 - Centro Portugal Regional Operational Programme (Centro2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund.



Centre for Mechanical Technology Automation (TEMA), Department of Mechanical Engineering, University of Aveiro

The Centre for Mechanical Technology and Automation (TEMA), active since 1996, was created with the main mission of excelling in scientific and technological excellence according to the needs of Portuguese society and its industries.

Nowadays, TEMA addresses the major competitive challenges faced by manufacturing and process industries worldwide, focusing on automation, productivity, and optimization. Recognising the importance of both scientific and societal challenges, TEMA disseminates its research in high-impact journals and engages in international projects and networks. While rooted in traditional mechanical engineering, TEMA evolves towards emerging fields like nanotechnology, sustainable engineering, and artificial intelligence, ensuring comprehensive, multidisciplinary research aligned with industry and societal needs.

MISSION

Create, implement, and disseminate scientific and technological knowledge to develop, innovate, and apply solutions in mechanical engineering and related disciplines while actively collaborating with industries. Anticipate and address the challenges of a global society.

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We aim to be at the forefront of technological development and strengthen our interventive role as a multidisciplinary research unit in the field of mechanical engineering and related disciplines. Foster the development of a global scientific culture and elevate students' engineering and science skills to a higher level. Encourage companies to engage in research and integrate doctorates into their workforce to stimulate innovation within the industrial sector.

RESEARCH

TEMA is focused on current societal challenges and upcoming global requirements, translated into three main mobilising programmes (MP): MP1 (Sustainable Manufacturing Solutions); MP2 (Techniques for wellbeing) and MP3 (Research Infrastructure), involving TEMA's members as one coherent group. MP1 is focused on the development and innovation of manufacturing engineering and technologies, with subsequent industrial applications. It is intended to increase productivity, improve products' quality, and reduce waste in production processes. The strategy of the MP2 aims to increase the quality of life in society by means of engineering systems, focusing on people and their needs. MP3 aims at a rational and efficient management of TEMA's material and human resources and its vast array of scientific equipment in a large diversity of areas available to society, making the research infrastructure an "open facility" for several (academic, research, and industry) end-users.

TEMA also works on the new Intelligent Systems Associate Laboratory. TEMA assisted in founding LASI, a 13-research unit consortium. (<https://lasi-research.pt/>).



Dr. Paula Alexandrina de Aguiar Pereira Marques
Coordinator of the Centre for Mechanical Technology and Automation (TEMA)



Recovery and Resilience Plan (PRR), Portugal

The Recovery and Resilience Plan (PRR) is a national application program, with an execution period until 2026, which aims to implement a set of reforms and investments aimed at restoring sustained economic growth, after the pandemic, reinforcing the objective of convergence with Europe over the next decade.

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Notes

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