

2nd International Conference on Nanotechnology Research and Innovation

November 19-22, 2024 University of Aveiro, Portugal Book of Abstracts





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Title

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Editors

Igor Bdikin Gil Alberto Batista Gonçalves Milan Vukšić Martina Kocijan

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2nd International Conference on Nanotechnology Research and Innovation, University of Aveiro, Portugal, November 19-22, 2024 (ICNTRI-2024)

ICNTRI-2024 looks for significant Modern Problems of Nanomaterials Research and Innovation, 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 Nanotechnology science theories, modelling, experiments, industrial implementations.

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ICNTRI2024 program

November 19, 2024 (Tuesday)

	November 13	, ``	• /
Auditorium 1 AMAT-2024 2 nd Workshop on ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES 19 November 2024, Aveiro, Portugal		Auditorium 2 WMTER-2024 3 rd International Workshop on "Modern Trends in Energy Research" 19 November 2024, Aveiro, Portugal	
9.00 - 9:30		9.00 - 9:20	Session Chair: Francisco Loureiro D. Pukazhselvan (welcome address and keynote lecture) TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal Title: Introduction to energy crisis and probable solutions
9.30 - 9:35	WELCOME ADDRESS Dr. Indrani Coondoo	09:20 10:45	Bruno Melo (plenary lecture) Department of Physics, University of Aveiro, Portugal Title: Solid acid composites as electrolytes for intermediate temperature fuel cells
09:35 _ 10:15	Chair: Indrani Coondoo Plenary Lecture Prof. Anil Kumar Department of Mechanical Engineering, Delhi Technological University, Delhi, India	09:45 10:00	Olena Okhay (Invited talk) TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal Title: Supercapacitor electrodes based on reduced graphene oxide by various methods
	Advancement in Energy Storage Materials Integrated Solar Drying Systems	10:00 _ 10:15	Ihsan Çaha (Invited talk) International Iberian Nanotechnology Laboratory, Braga, Portugal Title: Multi-Scale Characterization of NMC111 Cathodes for Li-ion Batteries: From Atomic Structure to Electrode Architecture with 4D STEM and FIB-SEM

10:15 _ 10:45	Plenary Lecture Prof. Majid Taghavi Department of Bioengineering, Imperial College London, London, UK Artificial muscles with extended functions for monolithic medical robots	10:30 _ 10:50	Session Chair: Vanessa Graca Sathishkumar Duraisami (Invited talk) TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal <i>Title: Optimisation of electron beam</i> <i>welding parameters for copper pipe joints</i> <i>in heat pump systems</i>
10:45 _ 11:30	Plenary Lecture Prof. Satyaprakash Sahoo Laboratory for Low Dimensional Materials, Institute of Physics, Bhubaneswar, India	10:50 – 11:15	Fausthon Fred da Silva (Invited talk)Chemistry Department, Federal University ofParaíba, BrazilTitle: Boosting the Electrocatalytic Activityof Metal-Organic Frameworks DerivedMetal-Organic Frameworks DerivedMetal-Oxide Nanoparticles in OxygenEvolution Reaction
	Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai, India Emerging 2D quantum materials for brain-inspired neuromorphic computing applications	11:15 _ 11:30	Alfredo S. B. Luemba (Invited talk) Department of Mechanical Engineering, University of Aveiro, Portugal Title: Development of novel proton- conducting materials for ceramic fuel cells/electrolyzers
11:30 _ 12:00	Chair: Ajeet Kumar Dr. Sugato Hajra Daegu Gyeongbuk Institute of Science and Technology, Daegu, South Korea Self-Powered Sensors using Triboelectrification Keynote talk	11:30 _ 11:50	Session Chair: Laura Holz Sivabalan Maniam Sivasankar (Invited talk) Department of Physics, i3N, University of Aveiro, Portugal Title: Interface and surface engineering of CIGS films to improve cell performance
12:00 _ 12:30	Dr. Daniela V. Lopes CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Aveiro, Portugal Advancements in alkaline electrolysis for sustainable steelmaking technology and	11:50 _ 12:05	Lara F. Almeida Paiva (Invited talk) TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal Title: A robust hydrothermal synthesis method of NH ₄ Zr ₂ (PO ₄) ₃ , a precursor for HZr ₂ (PO ₄) ₃ proton conductor
	emerging hydrogen electrocatalysts Keynote talk	12:05 _ 12:30	Vivek Shukla (Invited talk) Centre for Hydrogen Energy Materials, Korea Institute of Science and Technology, Seoul, 02792, Republic of Korea Title: Hydrogen sorption characteristics of Ti-Al-O ternary system

12:30 -		Lunch	
14:00 Auditorium 1 AMAT-2024 2 nd Workshop on ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES 19 November 2024, Aveiro, Portugal		Auditorium 2 WNCBM-2024 3 rd Workshop New Challenges of Bionanomaterials: Science, Technology, Application University of Aveiro, Portugal, 19 November 2024	
14.00 - 14:15	Chair: Indrani Coondoo Tiago Rodrigues Physics Center of Minho and Porto Universities (CF-UM-UP), University of Minho, Campus de Gualtar, Braga, Portugal Laboratory of Physics for Materials and Emergent Technologies, LapMET, University of Minho, Braga, Portugal Strain-Driven Polar Topologies in SrTiO ₃ - ô Thin Films Oral presentation	14.00 - 14:20	CHAIR: Dr. Igor Bdikin Dr. Gil Gonçalves Pioneering New Frontiers in biomedicine with Carbon-Based Nanomaterials Centre for Mechanical Technology and Automation (TEMA)-University of Aveiro, Portugal
14:15 - 14:30	Sunny Choudhary Department of Physics, University of Puerto Rico at Río Piedras, San Juan, USA Encapsulation Engineering of Sulfur into Magnesium Oxide for High Energy Density Li–S Batteries Oral presentation	14.20 - 14:45	CHAIR: Dr. Gil Gonçalves Dr. Igor Bdikin Atomic Force Microscopy Methods for Characterization of Organic Materials Centre for Mechanical Technology and Automation (TEMA)-University of Aveiro, Portugal
14:30 - 14:45	Noelle C. Zanini Department of Materials and Ceramic Engineering, CICECO – Aveiro Institute of Materials, University of Aveiro, Aveiro, Portugal Dynamic Response of Lead-free Composite Flexible Generator for Sustainable Blue Energy Solutions Oral presentation	14:45 - 14:55	Duarte Almeida Microfluidic production of multifunctional nanocomposites for lithium-based neutron capture therapy TEMA – Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro

Degra	um 1 WCSDOCR-2024 orkshop on Challenges and Strategies in dation of Organic Contaminants Research AALL MOLECULES, BIG PROBLEMS University of Rijeka, Croatia 19 November, 2024	
15:00 - 15:10	WELCOME ADDRESS Prof. Ivna Kavre Piltaver Dr. Matejka Podlogar, Dr. Martina Kocijan CHAIR: MSc. Tina Radošević	
15:10 - 15:30	MSc Daria Jardas Babić Faculty of Physics and Centre for Micro- and Nanosciences and Technologies, University of Rijeka, Croatia <i>Title:</i> Atomic Layer Deposition of Semiconductor Thin Films for Photocatalytic Applications	
15:30 - 15:50	CHAIR: MSc. Tina Radošević Prof. Aleš Omerzu Faculty of Physics and Centre for Micro- and Nanosciences and Technologies, University of Rijeka, Croatia <i>Title:</i> Thin ZnO films prepared by plasma- enhanced atomic layer deposition (PEALD) for future photocatalytic applications	
15:50 - 16:00	Coffee break	
16:00 - 16:20	CHAIR: Dr. Martina Kocijan Dr. Matejka Podlogar Department for Nanostructured Materials, Jožef Stefan Institute, Ljubljana, Slovenia <i>Title:</i> Modifying the defect population in ZnO nanorods through solvothermal synthesis for enhanced photocatalytic performance	
16:20 - 16:40	Dr. Marija Egerić Vinča Institute of Nuclear Sciences, Beograd, Serbia <i>Title:</i> Degradation of organic pollutants by gamma irradiation: progress in wastewater treatment	
16:40 - 17:00	Final discussion and comments	

November 20, 2024 (Wednesday)

	International Conference on Nanotechnology Research and Innovation (ICNTRI-2024) (online)		
9:00- 9:10	Auditorium 1 WELCOME ADDRESS: Dr. Igor Bdikin, Prof. Dr. Vikram Uttam Pandit, Prof. Dr. Gunnar Suchaneck, Dr. Gil Alberto Batista Gonçalves		
9:10- 9:40	CHAIR: Prof. Dr. Ricardo Pinto, Prof. Dr. Neeraj Panwar Session: New Materials and Advanced Materials Plenary Lecture Prof. Dr. Paula Ferreira Porous Foams of Caffeic Acid-Modified Reduced Graphene Oxide for Water Purification Department of Materials and Ceramic Engineering, CICECO – Aveiro Institute of Materials, University of Aveiro, 3810–193 Aveiro, Portugal		
9:40- 10:00	Session: Thin Films <i>Keynote talk</i> Dr. Ana Violeta Girão (I10) Boron Doped-Diamond Electrodes for Green Hydrogen Production via Electrolysis DEMaC – CICECO – University of Aveiro, Campus de Santiago, Aveiro, Portugal		
10:00- 10:15	Session: Environmental Friendly Materials Cátia Venâncio (O11) Assessment of the potential ecotoxicity of carbon and wood fibers targeting its incorporation into new products Center for Environmental and Marine Studies, Department of Biology, University of Aveiro, Aveiro, Portugal		
10:15- 10:30	Coffee break		
10:30- 11:00	Session: Hydrogen and Fuel Cell Science Plenary Lecture Prof. Dr. Domingo Pérez-Coll Electrical transport components in protonic ceramic conductors Instituto de Cerámica y Vidrio (ICV), CSIC, C/ Kelsen 5, Cantoblanco, Madrid, Spain		

11:00- 11:20	Session: Nanotechnology Prof. Dr. Lyubomira Radeva (O1) Double loading of doxorubicin and resveratrol in composite nanogels – a new strategy for alleviating neurotoxicity of doxorubicin Faculty of Pharmacy, Medical University of Sofia, 2 Dunav Str., 1000 Sofia, Bulgaria			
11:20- 11:45	Session: Thin Films Keynote talk Prof. Dr. Ivna Kavre Piltaver (I12) Tailoring Photocatalytic Performance in ZnO Films: Effects of Copper Doping and ALD Hot Source Temperature Faculty of Physics, University of Rijeka, Croatia Center for Micro- and Nanosciences and Technologies, University of Rijeka, Croatia			
11:45- 12:00	Session: Biocomposites Mahsa HEİDARNEJAD (O3) Synthesis and Characterization of Chitosan-Gelatin Biocomposite Wound Dressing with Alchemilla ellenbergiana Extract Sakarya University, Institute of Natural Sciences, Department of Chemistry, 54187, Sakarya, Turkiye Sakarya University, Biomaterials, Energy, Photocatalysis, Enzyme Technology, Nano & Advanced Materials, Additive Manufacturing, Environmental Applications and Sustainability Research & Development Group (BIOENAMS R&D Group), 54050 Sakarya, Turkiye			
12:00- 12:15	Session: Materials Science Esra ÇAKAR (O19) Synthesis and Characterization of Ag/Ag3VO4@rGO Nanocomposite Photocatalysts for Photocatalyti Food Dye Degradation Sakarya University, Institute of Natural Sciences, Department of Chemistry, 54187, Sakarya, Turkiye. Sakarya University, Biomaterials, Energy, Photocatalysis, Enzyme Technology, Nano & Advanced Materials, Additive Manufacturing, Environmental Applications and Sustainability Research & Development Group (BIOENAMS R&D Group), 54050 Sakarya, Turkiye			
12:15- 12:30	Session: Polymeric Composites Tao Cheng (O29) Bacterial cellulose reinforced mechanical robustness and self-repairable polyurethane composites with dual-dynamic bonds School of Materials and Energy, University of Electronic Science and Technology of China, Chengdu 610054, P. R. China			
12:30- 14:00	Lunch			

14:00- 14:15	CHAIR: Dr. Vanessa Graça, Dr. Francisco Loureiro Session: Stimuli Responsive Biomaterials Selen Şakar (O15) Synthesis and in vitro drug release of gentamicin-loaded gelatin-chitosan hydrogel Sakarya University, Institute of Natural Sciences, Department of Chemistry, 54187, Sakarya, Turkiye Sakarya University, Biomaterials, Energy, Photocatalysis, Enzyme Technology, Nano & Advanced Materials, Additive Manufacturing, Environmental Applications and Sustainability Research & Development Group (BIOENAMS R&D Group), 54050 Sakarya, Turkiye
14:15- 14:35	Session: New Methods of Modeling Properties Materials <i>Keynote talk</i> Dr. Anuraag Gaddam (I17) Investigation of Phosphate Nano-Clusters in Bioactive Glasses by Advanced Solid-State NMR <i>CICECO-Aveiro Institute of Materials, Department of Chemistry University of Aveiro, Aveiro, 3810-193,</i> <i>Portugal</i>
14:35- 14:50	Session: Thin Films LABLALI Mohammed (O5) Deposition rates and annealing effects on the growth of Nb thin film on Cu substrate: Molecular dynamic simulation Laboratory of Condensed Matter, Faculty of Science Ben M'Sick, University Hassan II of Casablanca, Morocco
14:50- 15:10	Session: New Energy Materials <i>Keynote talk</i> Dr. D. Pukazhselvan (I11) A novel cobalt trapped carbon-nitrogen 3D filamental structure as a potential anode active material for Li ion batteries <i>TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering,</i> <i>University of Aveiro, 3810-193 Aveiro, Portugal</i> <i>LASI - Intelligent Systems Associate Laboratory, 4800-058 Guimarães, Portugal</i>
15:10- 15:25	Session: Optical/Electronic/Magnetic materials Dr. Yagmur Pirincci Tok (O2) Investigation of in vitro drug release studies and antibacterial properties of the Fe3O4@TA@CHL drug delivery system Kocaeli Health and Technology University, Faculty of Pharmacy, Department of Toxicology, Kocaeli, Turkiye
15:25- 15:40	Coffee break
15:40- 16:00	Session: Optical/Electronic/Magnetic Materials <i>Keynote talk</i> Dr. Suresh Kumar Jakka (I19) Optical Gas Sensing Using Rare Earth Ion-Doped Glass Matrices <i>I3N-Department of Physics, University of Aveiro, Aveiro, Portugal</i>

16:00-	Session: Optical/Electronic/Magnetic Materials Keynote talk
16:20	Dr. Pavani Krishnapuram (120) Luminescence thermometry based on Rare earth spectroscopy I3N-Department of Physics, University of Aveiro, Aveiro, Portugal
16:20- 16:40	Session: Hydrogen and Fuel cell science Celina Fernandes (O24) An effective sealing method for planar solid oxide fuel cells using compressed vermiculite <i>LEPABE, Faculdade de Engenharia, Universidade do Porto, rua Dr. Roberto Frias, 4200-465 Porto, Portugal.</i> <i>ALICE – Associated Laboratory in Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr.</i> <i>Roberto Frias, 4200-465 Porto, Portugal</i>
	Session: Hydrogen and Fuel Cell Science
16:40- 17:00	Maxwell F.L.Garcia (O14) Solution-blown spun cobalt oxide nanofibers as electrocatalysts with enhanced oxygen evolution reaction activity Laboratory of Materials Technology, Department of Materials Engineering, Federal University of Campina Grande, Campina Grande, Brazil TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal
17:00-	Session: Nanotechnology Keynote talk
17:20	Dr. E.Venkata Ramana (122) Exploring fluorite ferroelectrics: pathways to innovative applications I3N, Department of Physics, University of Aveiro, Aveiro 3810-193, Portugal
	Session: Hydrogen and Fuel Cell Science Dr. Allan J. M. Araújo (O13)
17:20-	Overcoming oxygen surface diffusion limitations in lanthanum nickelate Ruddlesden-Popper
17:40	electrodes via praseodymium oxide infiltration for Solid Oxide Cells
	TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering,
	University of Aveiro, 3810-193 Aveiro, Portugal

November 21, 2024 (Thursday)

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	International Conference on Nanotechnology Research and Innovation (ICNTRI-2024) (online)
8:45- 9:00	CHAIR: Dr. Laura Holz, Dr. Gil Gonçalves Session: New Energy Materials Guo-Tao Xiang (O27) Flexible Solid-State Supercapacitors and Organic Ion Hydrogel Sensors for Self-Powered Smart Sensing Applications School of Materials and Energy, University of Electronic Science and Technology of China, Chengdu 610054, P. R. China
9:00- 9:20	Session: Materials Science Prof. Dr. Xiangnan Pan (O31) Characteristic nanostructure and its role in ductile and fatigue failure of metallic materials <i>LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, P. R. China</i>
9:20- 10:00	Session: Thin films Plenary Lecture Prof. Dr. Vincent Ball Electrochemical Design of Carbon-Based Functional Materials from Allomelanin Precursors with Dual Anti-Oxidant, Anti-Bacterial and other Properties Unité Mixte de Recherche 1121, « Biomatériaux et Bioingénierie », Institut National de la Santé et de la Recherche Médicale, 1 Rue Joseph Boeckel, Strasbourg,France Faculté de Chirurgie Dentaire, Université de Strasbourg, Strasbourg, France
10:00- 10:20	Coffee break
10:20- 10:40	Session: Composites <i>Keynote talk</i> Prof. Dr. Neeraj Panwar (I5) Non-volatile resistive switching behavior of Ag/PVA-graphene oxide/Ag device Department of Physics, Central University of Rajasthan, Ajmer, INDIA Department of Physics, Chaudhary Charan Singh University Meerut, Uttar Predesh, INDIA
10:40- 11:00	Session: Composites <i>Keynote talk</i> Prof. Dr. Vikram Pandit (I18) Photocatalytic applications of Stannous chloride and Pentacenequinone Composite system Haribhai V. Desai Arts, Science & Commerce College, Pune, India

11:00- 11:30	Session: Magnetic materials Plenary Lecture Prof. Dr. Gunnar Suchaneck Intergranular resistance and magnetoresistance of strontium ferromolybdate ceramics <i>Institute of Solid-State Electronics, TU Dresden, 01062 Dresden, Germany</i>
11:30- 12:00	Session: Polymer-ceramic composites Keynote talk Prof. Dr. Himansu Sekhar Nanda (I16) Ceramic reinforced Polymer Composites for Additive Manufacturing of Implants and Scaffolds Biomaterials and Biomanufacturing Laboratory (Formerly Biomedical Engineering and Technology Lab, Mechanical Engineering Discipline, PDPM Indian Institute of Information Technology, Design & Manufacturing, Jabalpur, Madhya Pradesh 482005, India Fused Filament Fabrication Laboratory, Mechanical Engineering Discipline, PDPM Indian Institute of Information Technology, Design & Manufacturing, Jabalpur, Madhya Pradesh 482005, India International Centre for Sustainable and Net Zero Technologies, PDPM Indian Institute of Information Technology, Design & Manufacturing, Jabalpur, Madhya Pradesh 482005, India
12:00- 12:20	Session: Materials science Dr. Martina Kocijan (O23) Atomic layer deposition of TiO2 thin films - enhanced tool for photocatalysis <i>Faculty of Physics and Centre for Micro- and Nanosciences and Technologies, University of Rijeka, Croatia</i>
12:20- 14:00	Lunch
14:00- 14:15	CHAIR: Dr. Venkata Eskilla, Dr. Martina Kocijan Session: Biomaterials Merve KEYF (O4) Innovative Application of Hydrogels in Drug Release Systems and 4D Printing Sakarya University, Biomedical Engineering, Institute of Natural Sciences, Esentepe Campus, 54187, Sakarya, Turkey
14:15- 14:30	Session: Biomaterials Tuğçe Neslihan DENİZ (O9) Drug delivery study of PCL and PVP-based hydrogels with shape memory property Sakarya University, Biomedical, Magnetic and Semiconductor Materials Research Center (BIMAS-RC), 54187, Sakarya, Turkey
14:30- 15:00	Session: Nanotechnology Keynote talk Prof. Dr. Musaab ZAROG (I6) Cubic silicon carbide for MEMS applications Sultan Qaboos University, Oman

15:00- 15:20	Session: Biomaterials Dilek BAYRAKDAR (O25) Production and Characterization of 4D Biomaterials for Drug Release Sakarya University, Biomedical Engineering, Institute of Natural Sciences, Esentepe Campus, 54187, Sakarya, Turkey
15:20- 15:30	Session: New Energy Materials Gintautas Jonkus (O21) Copper-based films obtained by anodization for supercapacitor applications Department of Physical Chemistry, Vilnius University, LT-03225 Vilnius, Lithuania
15:30- 16:00	Coffee break
16:00- 16:20	Session: Hydrogen and Fuel Cell Science <i>Keynote talk</i> Dr. Francisco Loureiro (I3) The future of decarbonization: how ammonia could lead the way <i>TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering,</i> <i>University of Aveiro, Aveiro, Portugal</i> <i>LASI - Intelligent Systems Associate Laboratory, Guimarães, Portugal</i>
16:20- 16:40	Session: Solid Oxide Fuel Cells <i>Keynote talk</i> Dr. Laura Holz (I4) Strontium iron molybdenum oxide (Sr2Fe1.5Mo0.5O6-δ) electrocatalyst for efficient nitrous oxide reduction in solid oxide fuel cells <i>TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering,</i> <i>University of Aveiro, 3810-193 Aveiro, Portugal.</i> <i>LASI - Intelligent Systems Associate Laboratory, Portugal</i>
16:40- 17:00	Session: Nanofluids <i>Keynote talk</i> Dr. Pavel Zelenovskii (I14) Unveiling water flows in diphenylalanine nanochannels Department of Physics and CICECO–Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal
17:00- 17:15	Session: Micro / Nano Materials Dr. Igor Bdikin (O18) Investigation of local properties and corrosion of copper and mild steel with different surface morphology <i>TEMA: Centre for Mechanical Technology and Automation, Department of Mechanical Engineering,</i> <i>University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal</i>

17:15- 17:30	Session: Micro / Nano Materials Laura Carvalho (O10) Rehabilitation of plastic-laden soils: a preliminary study using saprophytic fungi and polyethylene terephthalate Department of Biology, University of Aveiro, 3810-193, Portugal
17:30- 17:45	Session: Ceramics Miguel Vieira (O6) Development of thermoelectric composites with catalytic functionality <i>CICECO – Aveiro Institute of Materials, Department of Materials Engineering and Ceramics (DEMaC),</i> <i>University of Aveiro, 3810-193, Aveiro, Portugal</i>
17:45- 18:00	Session: Biomaterials Zinaida Shakel (O26) Innovative Skin Ageing Solution: Lipid Nanoparticles for Hyaluronic Acid Production LAQV, REQUIMTE, Faculty of Pharmacy, University of Porto, Portugal
18:00- 18:15	Session: Environmental Friendly Materials Adélio Fumo (O17) Prospects for electrodeposition of iron from mixed magnetite-metallic iron suspensions for steel production Department of Materials and Ceramic Engineering, CICECO – Aveiro Institute of Materials, University of Aveiro, 3810 - 193 Aveiro, Portugal Department of Chemistry, CICECO – Aveiro Institute of Materials, University of Aveiro, Portugal

November 22, 2024 (Friday)

	International Conference on Nanotechnology Research and Innovation (ICNTRI-2024) (online)		
	CHAIR: Dr. Igor Bdikin, Dr. Natália Barroca Session: Biomaterials		
8:40- 9:00	Prof. Dr. Meng-Yuan Dai (O30) De Novo Design of Modular Click-Peptide Chimeras for Immune Checkpoint Proteins Degradation Department of Gynecological Oncology, Zhongnan Hospital of Wuhan University, Wuhan, China		
	Session: Ceramics		
9:00- 9:20	<i>Keynote talk</i> Dr. Oleksandr Tkach (I9) Alternatively sintered of high-performance tunable dielectric Ba0.6Sr0.4TiO3 ceramics Department of Materials Engineering and Ceramics, CICECO – Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal		
9:20- 9:50	Session: Micro/nano materials <i>Keynote talk</i> Prof. Dr. Ana Luísa Daniel-da-Silva (I8) Biopolymer-Assisted Nanomaterial Surface Engineering: A Sustainable Approach to Water Treatment <i>Chemistry Dep./CICECO-Aveiro Institute of Materials, University of Aveiro, Aveiro, Portugal</i>		
9:50- 10:20	Session: Nanotechnology Prof. Dr. Erlong Wang (O22) The application of nanomaterials as the vaccine carrier in fish <i>College of Animal Science and Technology, Northwest A&F University, Yangling, Shaanxi 712100, China</i>		
10:20- 10:30	Coffee break		
10:30- 11:20	Session: Bio-Nanocomposites Plenary Lecture Prof. Dr. SABU THOMAS Circular Economy: New Opportunities in Sustainable Bio-Nanocomposites Mahatma Gandhi University, Kottayam, Kerala, India		
11:20- 11:50	Session: Biopolymers Dr. Pankaj Bharmoria (I7) Triplet-Triplet Annihilation Photon Upconversion Crystals Doped Bacterial Cellulose Composite Films as Recyclable Photonic Bioplastics Institute of Materials Science of Barcelona (ICMAB-CSIC)Universitat Autònoma de Barcelona Bellaterra, Barcelona, 08193, Spain		

	Session: Biomaterials
11:50- 12:05	Rabia Güzide AL (O8) Mechanical and Bioprosthesis Heart Valve Studies-A Review of Current Approaches <i>Biomedical Engineering, Institute of Natural Sciences, Sakarya University, Esentepe Campus, 54187 Sakarya,</i> <i>Turkey</i>
	Department of Electronics and Electronic Engineering, Dogus University, 34775 Istanbul, Turkey
	Session: Hydrogen and Fuel Cell Science Rui-dong Shi (O28)
12:05- 12:20	Minute-level Preparation as Ni(OH)2/NiS Hollow nanorods Heterostructure for Hydrogen Evolution Reaction in Alkaline
	School of Materials and Energy, University of Electronic Science and Technology of China, Chengdu 610054, P. R. China
12:20- 14:00	Lunch
	CHAIR: Dr. Alejandro Heredia Barbero, Dr. Pavel Zelenovskii Session: Biomaterials
14:00- 14:20	Dr. Burak ÜNLÜ (O7) Investigation of α-FeOOH/Dox/PEG system for controlled drug delivery Sakarya University, Biomedical, Magnetic and Semiconductor Materials Research Center (BIMAS-RC), 54187, Sakarya, Turkey
	Sakarya University, Biomaterials, Energy, Photocatalysis, Enzyme Technology, Nano and Advanced Materials, Additive Manufacturing, Environmental Applications and Sustainability Research and Development Group (BIOENAMS R&D Group), 54187, Sakarya, Turkey
	Session: Biomaterials Keynote talk
14:20- 14:40	Prof. Dr. Serbülent Türk (I2) Preparation and investigation of PEG based hydrogel systems containing CNTs with different functionalization ratios
	Sakarya University, Biomedical, Magnetic and Semiconductor Materials Research Center (BIMAS-RC), 54187, Sakarya, Turkey
	Session: New Energy Materials
14:40-	Plenary Lecture Dr. Andrei Kovalevsky
15:20	Innovative Composite MXene/Nickel Electrodes for Advancing Green Hydrogen Production by Alkaline Water Electrolysis
	CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal
	Session: Nanotechnology
15:20-	Keynote talk
15:40	Prof. Dr. Isabel Duarte (I15) Hybrid Structures based on Aluminum Foams for Enhanced Engineering Applications Department of Mechanical Engineering, TEMA - Centre for Mechanical Technology and Automation, LASI, University of Aveiro, 3810-193 Aveiro, Portugal
15:40- 16:00	Coffee break
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	Session: Nanofluids
16:00- 16:20	<i>Keynote talk</i> Prof. Dr. Abdelkadir Belhadj (I13)
	Heat Transfer Enhancement in Microchannels heat sinks MECACOMP Laboratory, Department of Mechanical Engineering, University of Tlemcen, Tlemcen, Algeria
16:20- 16:40	Dr. Zhi Jiang (O16)
	The Process of GaN-on-Diamond with Si Nano-intermediate Layer SAB Technology Departamento de Engenharia Mecânica, Universidade de Aveiro, Campus Universitário de Santiago, 3810- 193 Aveiro, Portugal
	Session: Protective Coatings and Corrosion of Materials Amira Gharbi (O20)
16:40- 17:00	Development of a novel efficient Ni-CeO2-Gr ternary nanocomposite coatings for Enhanced Corrosion and Wear Resistance
	Laboratory of Physics of Matter and Radiation (LPMR), Faculty of Science and Technology, University Mohamed Cherif Messaadia, BP 1553-41000 Souk Ahras, Algeria
	Session: Thin Films
17:00- 17:20	Keynote talk Prof. Dr. Aleksandr Bagmut (I1) Crystallization of amorphous laser condensates of hafnium and zirconium dioxides National Technical University "Kharkiv Polytechnic Institute", Kharkiv, Ukraine
	Session: Materials Science
17:20-	 Prof. Dr. Hassane MES-ADI (012) Heterogeneous interfaces effect on the mechanical behavior of Ag/Cu bilayers Laboratoire d'ingénierie des Procédés Informatiques et Mathématiques, ENSA de Khouribga, Université Sultan Moulay Slimane de Béni-Mellal, Maroc
17:40	Laboratoire de Physique de la Matière Condensée, Faculté des Sciences Ben M'Sik, Université Hassan II- Casablanca, B.P. 7955, Casablanca, Morocco Laboratoire Interdisciplinaire des Sciences Appliquées, Ecole Nationale des Sciences Appliquées Berrechid, Université Hassan I - Settat, Morocco
	Session: Protective Coatings and Corrosion of Materials
17:40- 18:00	Keynote talk
	Dr. Aleksey D. Lisenkov (121) Superhydrophobic Coatings on Laser-Structured Copper Oxide for Enhanced Corrosion Protection Department of Materials and Ceramics Engineering / CICECO, University of Aveiro, 3810-193, Aveiro, Portugal
18:00- 18:20	Conference Closing Ceremony

Plenary lectures

Intergranular resistance and magnetoresistance of strontium ferromolybdate ceramics <u>Gunnar Suchaneck *</u>

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Sr₂FeMoO₆₋₅ (SFMO) double perovskite is a promising candidate for room-temperature spintronic applications since it possesses a half-metallic character (with theoretically 100% spin polarization), a high Curie temperature of about 415 K, and a low-field magnetoresistance (LFMR) [1]. However, due to different synthesis conditions of ceramics as well as thin films, different mechanisms of electrical conductivity and magnetoresistance prevail. We start with the consideration of a granular metal network in which the metal grains are interconnected by insulating barriers [2]. In this case, ceramic grain boundary oxidation leads to the appearance of spin-polarized tunneling via an oxide barrier. Increasing the barrier width beyond the limit of thin tunneling barriers, inelastic hopping occurs via localized states within the barrier. Thereby, second- and third-order hopping conductances are characterized by $T^{4/3}$ and $T^{5/2}$ conductivity terms, respectively [3]. With further increase of the barrier width, the metallic-like conductivity disappears totally accompanied by an increase of the resistivity by about six orders of magnitude. The samples now exhibit a negative temperature coefficient of resistivity in the whole temperature region. Its resistivity behavior can be described in terms of the fluctuationinduced tunneling model, which converts near room temperature to a variable-range hopping conductivity mechanism. Here, the electron transport occurs through a thick barrier via more conductive chains of localized states in series with nanosized tunnel barriers between the grains. In the bulk limit and at high temperatures, inelastic hopping changes to variable range hopping as obtained experimentally [4]. The magnetic flux dependence of the tunneling barrier height was modeled by a series expansion, with empirical coefficients determined up to the second order. The magnetoresistance in SFMO ceramics is attributed to: (i) tunneling across intergrain barriers in granular ceramics, (ii) tunneling across intergrain nanocontacts in cold pressed and annealed at intermediate temperature granular ceramics.

References

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- [2] J. Inoue and S. Maekawa, Phys. Rev. B. 53, R11927 (1996).
- [3] Y. Xu, D. Ephron and M. R. Beasley, Phys. Rev. B. 52, 2843 (1995).
- [4] G. Suchaneck, et al., J. Alloys Comp. 860 158526 (2020).

Electrical transport components in protonic ceramic conductors Á. Triviño-Peláez, G. Heras-Juaristi, G.C. Mather, **D. Pérez-Coll**^{*}

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Proton-conducting ceramic materials have the potential to efficiently produce pure, dry hydrogen through steam electrolysis and convert hydrogen into electrical energy using fuel cells, particularly at high temperatures ranging from 600 to 900 °C [1]. However, extensive research into their transport properties under relevant conditions is necessary to advance promising technologies such as protonic ceramic fuel cells (PCFCs) and protonic ceramic electrolyser cells (PCECs). The performance of ion-conducting components in these devices is closely linked to the balance between ionic and electronic partial conductivities, the accurate measurement of which has long been recognised as critical for developing suitable materials and understanding their behaviour under specific operating conditions. Protonic ceramic perovskite conductors, typically derived from doped cerates and zirconates, exhibit high proton conductivity by absorbing water in hydrated environments. However, these materials often experience competition between various electrically charged species, leading to the presence of different electrical conduction components. This competition results in varying electrical responses depending on changes in oxygen and water-vapour partial pressures. In this context, we outline two methods for determining partial conductivities in systems with mixed protonic, oxide-ionic, and electronic conductivities. The first method involves measuring electromotive force while correcting for electrode polarisation when the materials are exposed to active gas gradients [2]. The second method examines electrical conductivity data under different oxygen and water-vapour partial pressure conditions, which are related to defect-chemistry analysis [3].

References

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- [2] D. Pérez-Coll, G. Heras-Juaristi, D.P. Fagg, G.C. Mather, *Journal of Power Sources*, **245**, 445-455 (2014).
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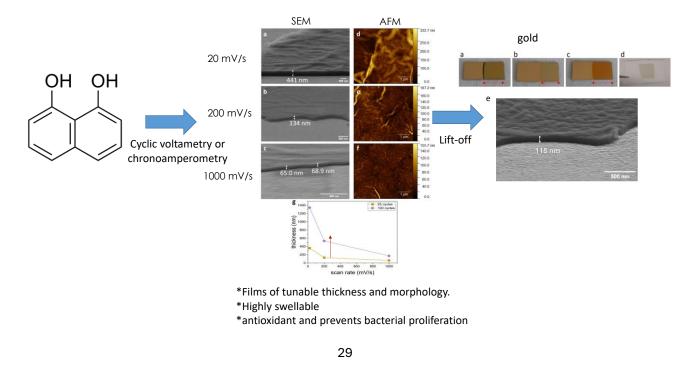
Acknowledgements

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Electrochemical Design of Carbon-Based Functional Materials from Allomelanin Precursors with Dual Anti-Oxidant, Anti-Bacterial and other Properties

Vincent BALL^{1,2,*}

The deposition of conformal films from redox-active biological molecules such as catechols, catechol amines and other polyphenols, has demonstrated great versatility in terms of the substrate used. Precursors of allomelanins, mainly found in fungi, have been largely overlooked as precursors for designing conformal and robust coatings. Moreover, their potential application for electrodeposition of films on conductive substrates has not yet been investigated. Here, the electrodeposition by cyclic voltammetry and chronoamperometry of 1,8-dihydroxynaphthalene (1,8-DHN), a precursor of allomelanin, onto gold and carbon electrodes and also onto Co-Cr alloys from aqueous solutions-ethanol mixtures yields films with potential sweep rate tunable thickness and swelling. The electrodeposition of 1,8-DHN will be compared to that of its isomers and will be shown to be unusual in the sense that films up to μ m thickness can be obtained without electrode passivation. The resulting films are antioxidant and the reservoir of antioxidant moieties is not limited to their surface but also extends into in the bulk of the film reflecting a high porosity and film swellability which was confirmed by means of spectroscopic ellipsometry. In addition, the films produced after a limited energy supply (in the potential window -1 V to +1 V vs Ag/AgCl) are strongly antimicrobial against two strains of *Pseudomonas aeruginosa* without further post- deposition treatment. In addition, their excellent mechanical properties (Young modulus around 600 Mpa in the wet state) allow them to be detached from their substrate as free-standing films (see Figure below), opening new avenues for diverse applications in biomedicine, energy storage, catalysis, sensing, and optoelectronics.



university of aveiro

Porous Foams of Caffeic Acid-Modified Reduced Graphene Oxide for Water Purification

Ana Barra^{1,2}, Avenancia Carvalho³, Cláudia B. Lopes³, Eduardo Ruiz-Hitzky², Cláudia Nunes¹, <u>Paula Ferreira</u>^{1,*}

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Graphene-based materials show great potential for water purification applications. In this study, we synthesized environmentally friendly sorbents through the hydrothermal reduction of graphene oxide (GO) in both the absence and presence of caffeic acid (CA), resulting in rGO and rGO_CA foams, respectively. A further modification with chitosan produced a third foam, designated CA_CS. Scanning electron microscopy revealed that the initially porous macrostructure of rGO became more compact after modification with CA or CA_CS. The specific surface area of the unmodified rGO foam reached up to 293 m²/g, with macropores ranging primarily between 1–170 µm. The Hg²⁺ removal efficiency of these rGO-based foams was tested under various conditions. The caffeic acid-modified foam exhibited the highest removal efficiency at pH 4–6, with a maximum sorption capacity of 2.79 mg/g, according to the Sips model. Kinetic analysis indicated that intraparticle diffusion and sorption were the rate-limiting steps. The foam's high sorption efficiency, low desorption rate, and effectiveness in complex water matrices, such as tap water, underscore the potential of rGO_CA as a highly effective material for Hg²⁺ removal from large volumes of water, with minimal solid waste for storage.

Acknowledgements

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university of aveiro tema centre for mechanical technology and automation

Innovative Composite MXene/Nickel Electrodes for Advancing Green Hydrogen Production by Alkaline Water Electrolysis

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Green hydrogen, produced through alkaline water electrolysis (AWE) powered by renewable energy, has the potential to dramatically reshape our energy systems by offering a clean and sustainable alternative to fossil fuels. As the demand for hydrogen grows, the development of innovative materials continues to fuel advancements in hydrogen-related technologies. MXenes, a class of 2D materials composed of transition metal carbides, nitrides, and carbonitrides, have shown great promise as electrocatalysts for water splitting. However, despite their potential, MXenes remain largely confined to academic research. Their industrial use is limited by challenges in their preparation and degradation in potential applications.

This study presents a straightforward and cost-effective method for developing composite electrodes designed for hydrogen production. Using titanium- and molybdenum-based MAX phases, along with MXene/Ni as functional components, several electrode configurations were prepared and tested. The approach employed an HF-free alkaline etching process, followed by comprehensive structural, microstructural, and electrochemical analysis. The results showed that the prepared electrodes exhibited remarkable electrochemical activity for the hydrogen evolution reaction (HER), in many cases outperforming the standard nickel electrodes currently used in industrial electrolysers. The possibility of further enhancing the electrochemical performance of the composite electrodes during the AWE process was also demonstrated.

Acknowledgements

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Circular Economy: New Opportunities in Sustainable Bio-Nanocomposites

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Green chemistry started for the search of benign methods for the development of nanoparticles from nature and their use in the field of antibacterial, antioxidant, and antitumor applications. Bio wastes are eco-friendly starting materials to produce typical nanoparticles with well-defined chemical composition, size, and morphology. Cellulose, starch, chitin and chitosan are the most abundant biopolymers around the world. All are under the polysaccharides family in which cellulose is one of the important structural components of the primary cell wall of green plants. Cellulose nanoparticles (fibers, crystals and whiskers) can be extracted from agro waste resources such as oil palm, jute, coir, bamboo, pineapple leafs, coir etc. These nanoparticles can be converted into smart and functional biomaterials by functionalization through chemical modifications (esterification, etherification, TEMPO oxidation, carboxylation and hydroxylation etc) due to presence of large amounts of hydroxyl group on the surface. The preparation of these nanoparticles includes both a series of chemical as well as mechanical treatments; crushing, grinding, alkali, bleaching and acid treatments. Transmission electron microscopy (TEM), scanning electron microscopy (SEM) and atomic force microscopy (AFM) are used to investigate the morphology of nanoscale biopolymers. Fourier transform infra-red spectroscopy (FTIR) and x ray diffraction (XRD) are being used to study the functional group changes, crystallographic texture of nanoscale biopolymers respectively. Since large quantities of oil palm bio wastes are produced annually, further utilization of palm cellulose, as functionalized materials is very much desired. The palm nano cellulose is currently obtained as aqueous suspensions which are used as reinforcing additives for high performance environment-friendly biodegradable polymer materials. These nanocomposites are being used as biomedical composites for drug/gene delivery, nano scaffolds in tissue engineering and cosmetic orthodontics. The reinforcing effect of these nanoparticles results from the formation of a percolating network based on hydrogen bonding forces. The incorporation of these palm based nanoparticles in several bio-based polymers have been discussed. The role of palm based nanoparticle dispersion, distribution, interfacial adhesion and orientation on the properties of the ecofriendly bio nanocomposites have been carefully evaluated.

Invited lectures

I1. Crystallization of amorphous laser condensates of hafnium and zirconium dioxides A. Bagmut

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Amorphous films of hafnium dioxide (HfO₂) and zirconium dioxide (ZrO₂) are formed on substrates at room temperature in the process of pulsed laser evaporation of Hf and Zr targets in an oxygen atmosphere. Irradiation of amorphous film with the electron beam initiates its crystallization. The transformation has one-stage character. The amorphous film of HfO₂ polymorphically passes into the crystalline one with monoclinic modification of HfO₂. According to the video recording data during crystallization of the film a single dendrite grows in the field of observation. The dendrite grows at the constant rate at the constant intensity of electron beam irradiation of the film. In this case *t*he crystalline fraction $x \sim t^2$. These structural and morphological characteristics qualitatively indicate the implementation of the dendritic polymorphous crystallization mode [1].

The amorphous film of ZrO_2 polymorphically passes into the crystalline one with cubic modification of ZrO_2 . According to the video recording data during crystallization of the film multiple crystals grows in the field of observation. Nucleation happens only at the beginning and growth takes place afterwards. Each crystal grows at the constant rate at the constant intensity of electron beam irradiation of the film. This nucleation mechanism would be identified as a Site-Saturate Nucleation (SSN) [2]. In this case $x(t) = 1-\exp(-kt^n)$. The Avrami exponent n = 2.03 (nearest integer = 2). It contains information about growth dimensionality (*N*). For site-saturated nucleation n = N. These structural and morphological characteristics qualitatively indicate the implementation of the island polymorphous crystallization mode.

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I2. Preparation and investigation of PEG based hydrogel systems containing CNTs with different functionalization ratios

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Hydrogel systems have emerged as a prominent area of studies in the recent research [1]. These versatile materials have found diverse applications in fields such as energy systems, biomaterials, and food coatings [2,3]. One of the key developments in this field involves the use of carbon nanotubes (CNT) as an additive to create conductive hydrogels due to their remarkable electrical conductivity [4]. To ensure effective interaction with polymers such as PEG and homogeneous distribution in polar solvents, polar groups are introduced onto the CNT surface.

This was achieved through a process of refluxing with acid in this study, resulting in CNT samples with varying degrees of functionalization. By creating homogeneous mixtures of functionalized CNT and PEG at different degrees, we have been able to form hydrogels through the freeze-thaw method. To assess the characteristics of the resulting materials, the zeta potentials of the obtained CNT solutions have been measured using UV-vis characterization, while the conductivities of the formed PEG-based hydrogels have been carefully evaluated.

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I3. The future of decarbonization: how ammonia could lead the way Vanessa C. D. Graça^{1,2}, Laura I. V. Holz^{1,2}, Allan J. M. Araújo^{1,2}, Duncan P. Fagg^{1,2}, <u>Francisco J. A. Loureiro^{1,2,*}</u>

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The EU's 2030 Climate and Energy Framework aims to significantly reduce CO₂ emissions through the development of innovative technologies for industries and processes [1]. Achieving this goal requires an urgent transition to a green economy, with a strong focus on the sustainable production of chemicals [2]. Ammonia (NH₃), a crucial chemical used globally in products like fertilizers and pharmaceuticals, plays a key role in this transition. However, its current industrial production via the Haber-Bosch process relies on high temperatures, pressures, and hydrogen from natural gas, resulting in significant CO₂ emissions [3]. A promising alternative is the electrochemical synthesis of NH₃ using Proton Ceramic Electrochemical Cells (PCECs), which enables ammonia production from renewable sources with minimal pollution [3]. This emerging technology offers a highly efficient and potentially disruptive pathway for producing one of the world's most essential chemicals in a more sustainable way [3].

Acknowledgments

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I4. Strontium iron molybdenum oxide (Sr₂Fe_{1.5}Mo_{0.5}O_{6-δ}) electrocatalyst for efficient nitrous oxide reduction in solid oxide fuel cells

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Nitrous oxide (N₂O) is a harmful environmental pollutant, necessitating the development of alternative abatement strategies [1]. In this study, we explored an electrochemical approach utilizing the mixed ionic-electronic conductor Sr₂Fe_{1.5}Mo_{0.5}O_{6-δ} (SFMO) as an electrocatalyst for N₂O reduction, within the temperature range of 600–800 °C and at ambient pressure, for application in Solid Oxide Fuel Cells (SOFCs). Electrochemical impedance spectroscopy (EIS) was used to investigate the electrode mechanism, revealing competition between reduction of O₂ and N₂O species, especially at lower temperatures where N₂O thermal decomposition is less efficient. The N₂O electroreduction was studied under polarization. Notably, the highest Faradaic efficiency (|Λ|) of 3.94 was observed at 600 °C for this reaction. The reversibility of the reaction mechanism was confirmed, as the reaction rate reverted to its open circuit value after current interruption. These findings suggest that the electrochemical promotion of N₂O reduction is a promising method for mitigating this environmentally harmful gas in SOFC systems.

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I5. Non-volatile resistive switching behavior of Ag/PVA-graphene oxide/Ag device Neeraj Panwar^{1,2}

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Non-volatile memory devices are getting significant attention from researchers worldwide in recent years due to their application in resistive random-access memory and neuromorphic computing. We have fabricated polyvinyl alcohol-graphene oxide (PVA-GO) composite as an active material for the resistive switching with different concentrations of GO (0.0, 0.1, 0.2, 0.3, 0.4, and 0.5 wt. % GO solution) dispersed in 5 wt. % PVA matrix in a 2:1 volume ratio. We demonstrate the non-volatile forming free resistive switching properties of Ag/PVA-GO/Ag devices. Structural properties of PVA-GO composites are established from the x-ray diffraction pattern, which indicates the complete dispersion of GO inside the PVA matrix. The Ag/PVA-GO-0.1 wt. % Ag device shows better bipolar resistive switching at $V_{\text{SET}} \sim 0.4$ V and V_{RESET} at ~ -0.8 V. This device indicates well-resolved two distinct states at a read voltage of 0.1 V in endurance and retention measurements. The fabricated device switches successfully tested for 2.5×10^3 cycles and retains its state for 3.36×10^3 s without any observable degradation. Furthermore, the non-volatile retention property was modeled using time series analysis. For this, Holt-Winter's exponential smoothing technique was utilized. Additionally, the charge-flux linkage characteristic shows the double-valued function, and time domain-charge and time domain-flux show asymmetric behaviors. The electrical conduction mechanism exhibits ohmic behavior in the entire region of the low resistance state and the lower voltage region of the high resistance state. In the high-voltage region of the high resistance state, the space charge-limited conduction mechanism is observed. The resistive switching behavior is explained with the help of an appropriate model.

I6. Cubic silicon carbide for MEMS applications <u>Musaab Zarog</u>

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Cubic silicon carbide (3C-SiC) has emerged as a highly promising material for microelectromechanical systems (MEMS) applications due to its exceptional mechanical, electrical, and thermal properties. This review provides a comprehensive analysis of the key attributes of 3C-SiC that make it an ideal candidate for MEMS devices, including its wide bandgap, high breakdown voltage, excellent thermal conductivity, and superior chemical and mechanical stability, particularly in harsh environments. The paper discusses the material's performance in various MEMS applications, such as pressure sensors, accelerometers, and resonators, where it outperforms traditional silicon-based devices in terms of reliability and durability. Challenges such as residual stress, wafer quality, and high-temperature processing are also explored, along with potential strategies to address these issues. By reviewing the current state of research and development, this paper highlights the potential of cubic silicon carbide to revolutionize MEMS technologies, especially in high-temperature, high-power, and corrosive environments.

I7. Triplet-Triplet Annihilation Photon Upconversion Crystals Doped Bacterial Cellulose Composite Films as Recyclable Photonic Bioplastics

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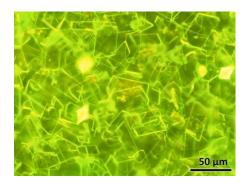
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Abstract: Biopolymers currently utilized as substitutes for synthetic polymers in photonics applications are predominantly confined to linear optical color responses.^[1] This work expands their applications in nonlinear optics by integrating with triplet-triplet annihilation photon upconversion (TTA-UC) crystals. TTA-UC converts two low-energy photons into one high-energy photon and has applications in photon harvesting and storage.^[2] A photon upconverting biomaterial is prepared by cultivating Pd(II) meso-tetraphenyl tetrabenzoporphine : 9,10-diphenyl anthracene (sensitizer: annihilator) crystals on bacterial cellulose



hydrogel that serves both as host and template for the crystallization of photon upconversion chromophores for the first time. Coating with gelatin improves the material's optical transparency by adjusting the refractive indices. The prepared material shows an upconversion of 633 nm red light to 443 nm blue light, indicated by quadratic to linear dependence on excitation power density (non-linearly). Notably, components of this material are physically dis-assembled to retrieve 66±1% of annihilator, at the end of life. Whereas, the residual clean biomass is subjected to biodegradation, showcasing the sustainability of the developed photonics material.^[2]

Figure 1 – Photon upconverting crystals embedded in bacterial cellulose-gelatin film

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I8. Biopolymer-Assisted Nanomaterial Surface Engineering: A Sustainable Approach to Water Treatment <u>Ana L. Daniel-da-Silva</u>*

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Access to clean water is essential for maintaining global health and driving economic progress. However, numerous emerging contaminants are frequently found in sources of drinking water, effluents from treatment facilities, and natural bodies of water, often at concentrations that threaten public and ecological health.

Nanotechnology has created new possibilities for improving the efficiency of water purification and wastewater reuse through the development of nanomaterials engineered for pollutant adsorption.¹ These nanomaterials feature high specific surface areas and distinct surface properties, such as tunable surface chemistry, which are advantageous for water treatment and environmental remediation. Ideally, an adsorbent material used in water purification should meet several criteria, including specificity for target contaminants, high adsorption capacity, rapid uptake, cost-effectiveness, non-toxicity, reusability, and ease of separation from the treated water. A simple combination of biopolymers with magnetic iron oxide nanoparticles can satisfy low toxicity and easy magnetic separation requirements. Nevertheless, careful surface design of the nanoparticles is essential to achieve specificity, enhanced adsorption capacity, and reusability. Herein, various chemical strategies for nanoparticle surface modification will be discussed, with an emphasis on systems developed for specific water treatment applications. Special attention will be given to the rational design of magnetic nanomaterials functionalized with biopolymers, aimed at developing advanced nanosorbents with high adsorption performance and reusability.^{2,3}

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I9. Alternatively sintered of high-performance tunable dielectric Ba_{0.6}Sr_{0.4}TiO₃ ceramics

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Ba_{1-x}Sr_xTiO₃ (BST) is a vital dielectric material in tunable devices for modern wireless communication technologies, owing to high dielectric tunability and low dielectric loss. However, conventional processing of BST ceramics requires a high sintering temperature of up to 1500 °C [1], arising interest in alternative sintering methods [2,3]. Here, the feasibility of using cold sintering process (CSP) and Flash sintering (FS) to process Ba0.6Sr0.4TiO3 ceramics, resulting in a significant decrease in the furnace temperature and reduction in the sintering process time, is demonstrated. The dielectric permittivity with over 10% tunability at room temperature under 15 kV/cm and with only ±7.1% variation over a temperature range of -90 °C to 85 °C, satisfying requirements to capacitor X5R grade, was obtained on 90% dense BST ceramics cold sintered at 350 °C for 4 h with Ba(OH)₂ as a flux [2]. BST ceramics with the density of 92% were obtained by FS at 1000 °C using isothermal conditions and multistep increase of current limit instead of constant heating rate and current single-step approach. Flash-sintered BST exhibits about twice finer grain microstructure, twice lower dielectric permittivity and loss, and doubled communication quality factor, reaching ~10⁴ under 20 kV/cm electric field, at room temperature when compared to 94% dense BST ceramics conventionally sintered at 1350 °C [3]. These findings highlight the effectiveness of alternative methods for the rapid and hence energy-efficient sintering of electroceramics, also opening possibilities to enhance their performance for wider application.

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I10. Boron Doped-Diamond Electrodes for Green Hydrogen Production via Electrolysis

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The industrial sector is facing an energy transition targeting the introduction of carbon neutrality technologies, including green hydrogen production. Thus, the latter process requires further technological advances and at much lower cost. This work aimed to evaluate the hydrogen electrolysis process using boron-doped diamond (BDD) electrodes prepared by chemical vapor deposition (CVD). Silicon, tungsten and silicon nitride were used as substrates with silicon nitride being the most suitable one for mechanically more stable films. Electrochemical analysis enabled assessment of the electrochemical response of the produced BDD films. The assembly of an electrochemical cell for the electrolysis of water using BDD electrodes showed that these films have the capacity to produce around half the volume of gas produced by conventional electrodes.

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I11. A novel cobalt trapped carbon-nitrogen 3D filamental structure as a potential anode active material for Li ion batteries

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In recent years R & D in lithium-ion batteries garnered considerable momentum, and Li ion batteries started replacing hydrocarbon fuels in every sector across the world. To improve the energy density of Li ion batteries, a high focus is paid on the development of new high-capacity anode active materials [1]. For instance, the widely employed anode in the current day commercial Li-ion batteries, natural graphite, offers a theoretical capacity of 372 mAh/g, which needs to be improved. In view of this requirement [2], our current study presents the development of a cobalttrapped, three-dimensional nitrogen-doped carbon filament network (designated as Co-NC) as an alternate high capacity anode-active material for Li-ion batteries. To optimize the 3D Co-NC, initially a cobalt-based metal-organic framework, ZIF-67, was made and then this MOF structure was then subjected to pyrolysis treatment under nitrogen atmosphere at 500 °C. By using the asprepared structure as anode active material, we have developed Li ion half cell batteries (configuration: CR2032), with Li as counter electrode, Celgard 3501 as separator and 1M LiPF₆ at EC/DMC as electrolyte. Detailed galvanostatic charge / discharge tests revealed that Co-NC delivers 562 mAh/g capacity at the current density of 100 mA/g, which is roughly 10 times higher capacity as compared to the capacity delivered by the pure ZIF-67 under the same testing conditions (obtained capacity using pure ZIF-67 as anode: 55.5 mAh/g). A detailed postmortem study after 100 cycles was conducted on both ZIF-67 and Co-NC based batteries and it is found that both the structures are stable, and no structural degradation occurs over cycles. Electrochemical impedance spectroscopy analyses confirm that there is no significant aging induced resistance from electrolyte in both the batteries. However, we have evidence that capacitive resistance because of aging is higher in ZIF-67 based battery than in Co-NC employed battery. With these developments, we believe that Co-NC is a promising alternate anode for commercial Li ion batteries.

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I12. Tailoring Photocatalytic Performance in ZnO Films: Effects of Copper Doping and ALD Hot Source Temperature

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Industrial development has significantly contributed to environmental pollution, particularly through organic pollutants, highlighting the urgent need for global wastewater recycling. Over the past two decades, research has focused on photocatalytic degradation of pollutants in wastewater [1]. This process begins when a semiconductor absorbs light with energy greater than its band gap, creating free electrons and holes that react with oxygen or water on the surface, forming reactive species like superoxide anions and hydroxyl radicals [2]. These species oxidize organic materials into carbon dioxide, water, and mineral acids. Recently, ZnO has gained attention as a photocatalyst due to its thermal and mechanical stability, non-toxicity, and suitability for photocatalytic redox processes [3]. Research has explored its use in water purification, hydrogen production, and self-cleaning treatments. ZnO, a wide bandgap material, functions as an effective photocatalyst under UV light. Current research aims to modify its energy bandgap and enhance its ability to absorb visible light, typically through doping with transition metals. Copper is a particularly promising dopant, as it can substitute zinc in the lattice, creating oxygen vacancies that significantly influence the material's properties [4].

Photocatalytic efficiency is linked to the catalyst's surface area, with nanostructures like nanoparticles or nanorods offering high efficiency but prone to agglomeration and difficult removal. Polycrystalline thin films, with nanosized grains and large surface areas, are a promising alternative, as they can be coated on various substrates and easily recovered after use [5].

Several methods, including sol-gel dip-coating, spray pyrolysis, RF co-sputtering, etc. have been used to fabricate Cu-doped ZnO thin films for visible-light photocatalysis. Among these, atomic layer deposition (ALD) has emerged as a promising technique for growth of semiconducting or insulating thin films. This method has some unique properties and advantages compared to the other deposition techniques. Namely, ALD employs layer-by-layer growth of thin films, which enables accurate film thickness control and allows the deposit of conformal thin films on different substrates of various shapes and porosity [6]. While ALD-grown ZnO films have shown efficient UV photocatalytic

activity, the impact of copper doping on their performance under visible light remains to be thoroughly investigated.

We have used the ALD technique to synthesize thin ZnO films and Cu-doped ZnO films on flat silicon wafers. In our recent study, we investigated the effect of varying Cu concentrations on the structural, optical, electrical, and photocatalytic properties of ZnO films [7]. Furthermore, we will present new findings on the influence of hot source temperature on these properties in Cu-doped ZnO films synthesized via the ALD growth process.

To analyze the impact of Cu doping, we used scanning electron microscopy (SEM) and atomic force microscopy (AFM) to study the surface morphology and topology of the samples. Grazing incidence x-ray diffraction (GIXRD) was employed to assess crystallinity. X-ray photoelectron spectroscopy (XPS) and secondary ion mass spectrometry (SIMS) helped determine the chemical state and distribution of Cu atoms within the films. UV–vis spectroscopy was used to evaluate optical absorption in Cu-doped ZnO samples, and Hall effect measurements provided data on charge carrier concentration. Finally, photocatalytic activity was assessed by measuring the degradation rate of methylene blue (MB) in an aqueous solution under simulated solar radiation.

In summary, we examined the structural, optical, electrical, and photocatalytic properties of both pure ZnO films and ZnO films doped with Cu during the ALD process, varying the Cu concentration and hot source temperature. Our findings demonstrate that Cu doping successfully shifts the photocatalytic activity of ZnO films from UV to visible light. Additionally, increasing the hot source temperature produced films with altered surface morphology, crystal structure, and roughness, which significantly influence photocatalytic performance.

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I13. Heat Transfer Enhancement in Microchannels heat sinks Abdelkadir Belhadj^{1*}, Rachid Saim²

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This article provides numerically a study of forced convective flow inside microchannels and minichannels heat sinks for electronic devices cooling; Different geometries of microchannels are studied. The Navier–Stokes and energy equations are used to model the convective heat transfer process with the following assumptions: Twodimensional, incompressible, laminar and in steady state. The effect of gravity and other forms of body forces are negligible. The properties can be considered as constant because of the narrow temperature range. The continuity, momentum and energy equations for laminar flow are used to simulate the flow using Ansys Fluent.

The aim is to enhance heat transfer by laminar flow with a Reynolds number ranging from 150 to 1500. A significant enhancement in dynamic and thermal performances is observed, which improve the effect of the geometry on the dynamic parameters: friction coefficient increases with Reynolds number, and on the thermal parameters: Nusselt number and heat flow rate are improving in a remarkable way when Reynolds number increased.

Secondly, laminar forced convective flow of nanofluid-based water/Al2O3 in a twodimensional horizontal microchannel heat sink is investigated. The founding results showed that the use of nanofluid has enhanced the heat transfer in comparison with pure fluid, and the increasing of Al2O3 concentration enhances the thermal and dynamic parameters.

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I14. Unveiling water flows in diphenylalanine nanochannels P. Zelenovskii^{1,*}, M. Soares², C. Bornes³, S. Kopyl¹, L. Mafra², F. Figueiredo¹

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Properties of water confined in nanochannels essentially differ from a macroscopic bulk state. Ionic functional groups, covering the internal surface of peptide nanochannels, can modify water organization and behavior and additionally bias its properties. Study of such systems is of great fundamental and practical importance. In this work, we used a combination of single crystal X-ray diffraction, solid-state nuclear magnetic resonance (NMR) spectroscopy, and dynamic vapour sorption (DVS) measurements to analyse water motion inside self-assembling diphenylalanine (Phe-Phe, FF) nanochannels. We found the formation of two independent water flows: a conventional axial flow located around the nanotubes axis and a helical flow located near the peptide shell. These flows are independent of each other and their diffusion coefficients differ by several orders of magnitude. The molecular dynamics simulations have confirmed the trajectory of the helical flow being dictated by the screw-like distribution of the functional groups within the channel walls, while its flux is governed by external water vapour pressure.

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I15. Hybrid Structures based on Aluminum Foams for Enhanced Engineering Applications

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Hybrid structures based on aluminium foams represent an innovative class of lightweight materials, engineered to integrate the key benefits of aluminium foams—such as low density and high specific strength—with enhanced mechanical and functional properties tailored for demanding applications. These hybrid structures are developed by combining aluminium foams with complementary materials, such as polymers, which strategically fill the cellular pores of the aluminium foams. This approach creates multifunctional structures with improved mechanical, thermal, and acoustic properties, making them highly suitable for a range of engineering applications.

These hybrid structures were characterized using advanced material techniques, including uniaxial compression tests, X-ray microtomography, thermal analysis, fire and acoustic tests, and infrared thermography. These methods provided detailed insights into the structural integrity, thermal stability, and acoustic performance of the hybrid structures. Current research aims to enhance manufacturing processes and explore novel material combinations to broaden the potential of aluminium foam-based hybrid structures for engineering applications.

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I16. Ceramic reinforced Polymer Composites for Additive Manufacturing of Implants and Scaffolds

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Additive manufacturing (AM) has shown significant potential in biomanufacturing implants and scaffolds for tissue engineering. However, the high cost and lack of available medical grade feedstock hinders its wide application and remains a challenge. Fused filament fabrication (FFF) is an economical, commonly available yet powerful AM technique to produce customized implants and scaffolds using synthetic polymer filaments. To facilitate the wide application of FFF method in biomanufacturing, polymer infused custom filament has been proposed by researchers to effectively utilize the dual benefits of bioactive ceramics and biodegradable polymers. Here, we present two types of customized osteoconductive biodegradable composite filaments of optimal printability that can be used to 3d print bioactive bone scaffolds using any kind of FFF based 3d printer. We identified two osteoconductive ceramics i.e., calcium sulphate (CaS) and wollastonite powder (WPs) to develop highly loaded ceramic infused polymer composite filament. The objective of this study was to investigate the processibility of composite filaments with maximum ceramic content through FFF process to improve the mechanical, thermal, and biological performance of virgin polymers (Poly Lactic Acid (PLA) and PLA/Polycaprolactone (PCL) polymer blends) for tissue engineering applications. Composite ceramic reinforced polymer filaments were produced using chemical methods and melt compounding methods with CaS and WPs reaching upto 40wt %. CaS infused PLA composite filament exhibited enhanced thermal stability and marginal improvement in mechanical strength. The mechanical strength was improved by 29% at 20wt% of CaS. PLA-CaS solid specimens demonstrated biocompatibility and zero cytotoxicity when cultured with MC3T3E1 cells. The composite filaments are 3Dprinted for its use as bone scaffolds and bioresorbable screws for Anterior Cruciate Ligament (ACL) reconstruction. Similarly, WPs infused PLA/PCL composite filaments were 3d printed to porous scaffolds. The porous scaffolds had pores of 550µm with interconnectivity, porosity of over 50% and improved compressive strength (nearly 90%) compared to pristine PLA scaffolds). The flexural strength was remarkably improved at 40wt.% of WPs loading. The inclusion of WPs did not affect the thermal property of the scaffolds; however, inclusion of PCL in PLA reduced thermal stability. The biocompatibility test using MC3T3-E1 cells confirmed cell viability and early mineralization in pre-osteoblast cells suggesting suitability of these composite biomaterials for bone

tissue engineering application. The overall investigations highlight the potential of ceramic infused polymeric materials for biomanufacturing implants and scaffolds biomedical applications.

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I17. Investigation of Phosphate Nano-Clusters in Bioactive Glasses by Advanced Solid-State NMR

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Bioactive glasses (BGs) are renowned for their ability to bond with living tissues, making them highly suitable for applications in bone regeneration and tissue engineering. The incorporation of phosphate plays a pivotal role in their bioactivity, particularly in the nucleation of hydroxyapatite, a process that underpins the material's bone-bonding capability. It is well established that phosphate ions form nano-clusters within the glass matrix [1-3], yet the precise nature and organization of these clusters remain poorly understood. In this study, we employ advanced ³¹P Static Spin Echo Decay (SED) NMR combined with atomic simulations to investigate the structural characteristics of phosphate clustering in bioactive glasses. This approach provides critical insights into the size and distribution of phosphate nano-clusters, shedding that could shed light on their role in the material's bioactive behavior and hydroxyapatite formation. Our findings contribute to a deeper understanding of phosphate dynamics in BGs, offering valuable guidance for optimizing their design in biomedical applications.

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118. Photocatalytic applications of Stannous chloride and Pentacenequinone Composite system Vikram Pandit*

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Stannous chloride dehydrate (SnCl2.2H2O) and NH4OH were used in a hydrothermal reaction technique to create SnO2 nanoparticles. XRD, IR, UV, and FESEM were used to characterize the SnO2 nanoparticles. Tin has a tetragonal rutile structure and an average crystalline size of 4.5 nm, as indicated by the XRD findings spectrum, which primarily show oxygen and Tin peaks. FESEM micrographs demonstrate the flower-like structure of the produced SnO2. The XRD results show good crystallinity, and the produced SnO2 particles are homogeneous and consistent in size. This work illustrates the use of the hydrothermal reaction method to synthesize SnO2 nanoparticles. Because of their optical characteristics, band gaps of 3.6 eV and 3.37 eV, respectively, thermal stability, and photocatalytic activity, pentacenequienone and SnO2 were chosen as nanocomposite materials by employing cyclohexanedione and ortho-pthaldehyde as substrates 6.13 PQ.

I19. Optical Gas Sensing Using Rare Earth Ion-Doped Glass Matrices Suresh Kumar Jakka*

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This presentation is on the development of photoluminescent (PL) rare earth (RE³⁺) ion-doped glasses for highly sensitive gas detection. Glasses based on matrices such as silica, phosphate, tellurite, and chalcogenide, when doped with RE ions like europium (Eu³⁺), erbium (Er³⁺), and ytterbium (Yb³⁺), exhibit distinct optical emissions across the visible (VIS), infrared (IR), and mid-infrared (MIR) ranges, enabling versatile gas sensing applications. Eu³⁺-doped glasses emit at approximately 615 nm, making them effective for oxygen (O_2) detection due to the quenching of PL intensity in O_2 environments. Er³⁺-doped glasses, with emission around 1.5 µm, are suitable for carbon dioxide (CO_2) sensing, showing PL intensity variations proportional to CO_2 concentration. Yb³⁺-doped tellurite glasses, emitting near 1 μ m, are well-suited for sulfur dioxide (SO₂) detection, enhancing both sensitivity and selectivity. Additionally, Er³⁺ and Yb³⁺-doped chalcogenide glasses exhibit properties suitable for methane (CH₄) detection due to broad MIR transmission and a high refractive index. These materials can be fabricated into optical fibers, enabling remote, high-sensitivity gas sensing adaptable to harsh environmental conditions, supporting applications in environmental monitoring and industry. The study discusses glass properties, PL mechanisms, fabrication processes, and the operational principles of gas detection using these advanced materials.

I20. Luminescence thermometry based on Rare earth spectroscopy <u>K. Pavani</u>

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Diverse optical thermal sensing behavior of a thermally stable compounds from the Aurivillius famly, specifically bismuth lanthanum tungstate doped with Er³⁺/ Yb³⁺ phosphor prepared by solid-state reaction method is the focus of the present work. Various analytical techniques, including X-ray diffraction (XRD), Raman spectroscopy, diffuse reflectance spectroscopy (DRS), Fourier Transform Infra-red (FTIR ATR) and field emission scanning electron microscopy (FE-SEM), were employed to analyze the structural and morphological properties of the material. The results revealed that the material exhibited an iso-structural nature similar to the monoclinic high temperature phase (HT) of Bi₂WO₆. The DRS spectra displayed a broad band in lower wavelength region (200 - 475 nm), which was a combination of La-O charge transfer band, Bi³⁺ $({}^{1}S_{0} \rightarrow {}^{3}P_{1})$ and W-O LMCT band, with a bang gap of 2.2 eV. Temperature dependence of Upconversion (UC) bands in the visible region, corresponding to Er³⁺ (²H_{11/2}, ⁴S_{3/2}, ⁴F_{9/2} \rightarrow ⁴I_{15/2}); transitions was investigated in the temperature range of 15-300 K. The ratios of different UC band combinations were analyzed. Fluorescence intensity ratios (FIR) of thermally coupled (TCL) and non-thermally coupled (NTCL) levels were selected and validated using appropriate theoretical methods. Corresponding absolute (SA) and relative sensitivities (S_R) were estimated to compare the efficiency of different UC band combinations. In the present case of BLW: Er³⁺/Yb³⁺, S_R (1.01 % K⁻¹) associated with the TCL of Er³⁺ UC exhibited the highest sensitivity among all the NTCL combinations studied at 300 K.

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I21. Superhydrophobic Coatings on Laser-Structured Copper Oxide for Enhanced Corrosion Protection

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Surface wettability describes a liquid's ability to maintain contact with a solid surface, which is influenced by factors such as surface texture and chemical composition. Superhydrophobic surfaces as a critical focus, offering potential in diverse areas including microfluidic chips, oil-water separation devices, anti-icing coatings, liquid-repellent membranes, and micro-droplet manipulation systems.

Key to achieving desired wettability characteristics are structural roughness and surface chemistry, which have guided the development of numerous fabrication strategies. Femtosecond laser micromachining has proven especially effective in tailoring surface morphology and roughness, providing precise control over wettability. This study applies these principles to create superhydrophobic coatings on copper oxide surfaces, offering an innovative approach to corrosion-resistant, water-repellent materials.

The development of superhydrophobic coatings on copper oxide surfaces was explored to enhance corrosion resistance through hydrophobic film formation. Copper oxide layers, fabricated on copper plates using laser treatment, served as substrates for silane application. The laser process parameters optimized the formation of a controlled oxide layer, after which different silanes were applied from ethanol-based solutions. Both fluorinated and non-fluorinated silanes were tested, with fluorinated silanes providing superior hydrophobicity as demonstrated by contact angle measurements.

The study analyzed the effect of alkyl chain length in non-fluorinated silanes on hydrophobicity. Longer chains, such as hexadodecyltrietoxysilane, outperformed shorter alkyl groups, achieving more substantial water resistance. SEM imaging revealed the formation of organic structures on the copper oxide surface post-treatment, likely contributing to enhanced hydrophobicity by reinforcing the roughness and reducing water-solid contact. These findings underscore the critical role of surface morphology in superhydrophobic performance, where nanostructured layers effectively repel water.

Intended primarily for corrosion protection, these coatings could minimize water-induced degradation of copper surfaces, potentially improving their longevity in harsh environments. The study demonstrates the feasibility of achieving robust superhydrophobicity with careful control of silane chemistry and deposition conditions, offering valuable insights for environmentally conscious materials development in corrosion-resistant applications

I22. Exploring fluorite ferroelectrics: pathways to innovative applications

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To address greenhouse gas emissions from vapor-compression-based cooling technologies, there is a need to develop low-noise, environmentally friendly refrigerants. Electric field-induced cooling represents a promising alternative as it offers a fast, affordable, on-chip cooling solution that can be scaled to smaller dimensions. Nanostructures with switchable polarization near phase transitions can exhibit significant entropy changes, which can be finely tuned by adjusting material properties. Unlike bulk crystals, engineered ferroelectric heterostructures, such as epitaxial thin films, present notable advantages for integration into microelectronics, enabling higher efficiency and energy recovery strategies.

In this study, we developed and examined the caloric effects of ferroelectric oxide thin films. We evaluated detailed structural, microstructural, and physical properties, with indepth X-ray diffraction analysis confirming the oriented growth of oxide ferroelectrics with different lattice strains. Furthermore, varying doping concentrations in the materials displayed both positive and negative caloric properties due to compositional adjustments. We observed adiabatic temperature changes of up to 6 K in binary oxide nanostructures. These findings suggest that high-quality nanostructures with tailored lattice strain and dimensions hold potential as eco-friendly refrigerants, capable of efficient solid-state cooling under moderate external stimuli.

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Oral presentations

O1. Double loading of doxorubicin and resveratrol in composite nanogels – a new strategy for alleviating neurotoxicity of doxorubicin

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Doxorubicin treatment is known to induce significant neurotoxicity which complicates its safe use. The simultaneous loading of doxorubicin and antioxidant in nanosized drug delivery system could reduce neurotoxicity. The aim of the present study was to apply an innovative strategy for encapsulating the hydrophilic antitumor agent doxorubicin hydrochloride and the hydrophobic antioxidant resveratrol in nanogel particles. Nanogels are a type of nanoparticles that could improve the pharmacokinetic properties of the loaded drugs, provide passive targeting and increased selectivity [1,2]. However, the incorporation of hydrophobic drugs into such hydrophilic systems could be a challenge [3,4]. Thus, in order to increase the solubility of resveratrol a complex with hydroxypropylβ-cyclodextrin was first developed. Thereafter, the complex and doxorubicin were encapsulated into nanogels prepared from chitosan and bovine serum albumin via electrostatic gelation and heating. DLS analysis revealed small size of approx. 31 nm, PDI of 0.188 and 3-potential of + 51 mV. Transmission electron microscopy confirmed the small size and spherical shape of the particles. The successful encapsulation of both drugs into the composite nanogels was proved via IR-spectroscopy and XRD analyses. The encapsulation efficiency for doxorubicin was 73.3 % and for resveratrol 97.8 %. Furthermore, in vitro dissolution test showed a pH-dependent release, more pronounced in slightly acidic medium. The potential of the nanogel and simple solution of both drugs to reduce neurotoxicity of doxorubicin was evaluated in neuroblastoma SH-SY5Y cells. The results revealed that the encapsulated resveratrol exerted protective effect on the cells. Importantly, the treatment with the double loaded nanogel resulted in lower cytotoxicity compared to the solution of the drugs. Therefore, the double loaded composite system could be considered worthy of further investigation.

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O2. Investigation of *in vitro* drug release studies and antibacterial properties of the Fe₃O₄@TA@CHL drug delivery system Münteha Özsoy¹, <u>Yagmur Pirincci Tok</u>^{2,*}

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Introduction: Among nanomedicines, iron oxide nanoparticles (IONPs) are one of the most powerful tools for imaging applications, immunoassay, tissue repair, hyperthermia and drug delivery due to their numerous properties including small size, low toxicity, superparamagnetic and magnetic properties [1]. Because of their shape, roughness and surface properties, they are excellent candidates for interacting with bacteria and therefore have antimicrobial activity [2].

Methods: The synthesis of Fe_3O_4 magnetic nanoparticles (MNPs) and their subsequent modification with tannic acid (TA), followed by chloramphenicol (CHL) drug loading, were conducted based on established literature protocols [3]. The synthesized MNPs were characterized by XRD and FTIR. The loading and releasing of CHL were evaluated using UV-Vis spectroscopy at 275 nm.

Results: TA-functionalized iron oxide magnetic nanoparticles were synthesized successfully. The drug was loaded onto Fe3O4 MNPs and confirmed by XRD and FTIR characterization studies. *In vitro* drug release studies showed sustained release behavior.

Conclusion: In this study, Fe₃O₄ magnetic nanoparticles functionalized with TA were synthesized and loaded with CHL to increase antibacterial activity. Tannic acid offers advantages such as enhancing drug loading capacity and ensuring biocompatibility. Instead of penetrating multiple tissues, targeting CHL molecules to the desired tissue via magnetic iron oxide nanoparticles may offer great advantages.

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O3. Synthesis and Characterization of Chitosan-Gelatin Biocomposite Wound Dressing with *Alchemilla ellenbergiana* Extract

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Abstract

A wound is the inability of living tissue to maintain its function due to the deterioration of the structure of human skin for various reasons. The goal of wound care is to ensure the fastest possible tissue repair, to regulate the damaged skin structure, to prevent infection, to minimize wound discharge and edema, to reduce pain, and to achieve the best possible aesthetic appearance. In this study, a wound dressing has been designed to accelerate the healing process of cuts on the human body. The wound dressing is made using biocompatible, antimicrobial, oxygen-permeable, and biodegradable biocomposite materials such as chitosan and gelatin. As a unique feature, the hydrogel wound dressing includes an extract from the lion claw plant (*Alchemilla ellenbergiana*), which accelerates wound healing. The study was supported by characterization methods including SEM, FTIR, antimicrobial activity, swelling analysis, UV-VIS spectroscopy, and contact angle analysis.

Introduction

The scope of this study involves the development of a wound dressing that facilitates quicker and more hygienic closure of wounds. The wound dressing incorporates lion claw (*Alchemilla ellenbergiana*) to accelerate the healing process. Wound healing is a complex process that involves the interaction of many factors. The wound-healing effects of *Alchemilla* species are attributed to the tannins they contain, which possess anti-inflammatory and antimicrobial properties. Tannins can accelerate healing by tightening tissues and reducing bleeding. For this reason, *Alchemilla* species have traditionally been used to promote wound healing [1]. Various hydrogels are utilized in the fabrication of wound dressings. In this study, a hydrogel were produced using chitosangelatin biocomposite materials [2]. The materials used in the hydrogel production are biocompatible. The purpose of this wound dressing is to promote the rapid closure of non-healing wounds, making it a valuable tool in wound treatment.

Method

In this study, separate solutions of gelatin and chitosan were prepared. To the prepared chitosan solution, glycerol (0.15 mL) and Tween 80 (0.15 mL) were implemented and mixed for 30 minutes using a magnetic stirrer. Similarly, glycerol (0.35 mL) and Tween 80 (0.35 mL) were implemented

to the gelatin solution, which was then mixed at 50°C for 30 minutes using a magnetic stirrer. The resulting solutions were combined and stirred together at 40°C for 24 hours using a magnetic stirrer. Subsequently, 1.5 mL of a 0.25% glutaraldehyde solution was implemented to the gelatin and chitosan mixture, and the solution was stirred for 3 hours using a magnetic stirrer. Then, 2.5 mL of a 5% *Alchemilla ellenbergiana* extract was added to the solution and stirred homogeneously using a magnetic stirrer for 24 hours. After 24 hours, the homogeneous solution was transferred into Petri dishes and left to dry at room circumstances for 48 hours.

Results and Discussion

SEM analysis revealed that the *Alchemilla ellenbergiana* extract was incorporated into the formed pores, indicating a porous structure. FT-IR spectra showed distinct absorption peaks corresponding to *Alchemilla ellenbergiana*, chitosan, and gelatin, confirming the presence of all three components [3]. The light transmittance values of the extract were observed to decrease as the extract concentration increased, enhancing the UV barrier properties of the films. Additionally, light absorption values increased with higher extract concentrations. The water absorption analysis showed that the hydrogel film exhibited a standard absorption rate. The antimicrobial analysis demonstrated that the hydrogel film possesses antimicrobial properties. Thus, the chitosan-gelatin-*Alchemilla ellenbergiana* hydrogel film was found to be suitable for use as a wound dressing.

Conclusion

The produced chitosan-gelatin-*Alchemilla ellenbergiana* films were analyzed using scanning electron microscopy (SEM), Fourier-transform infrared (FT-IR) spectroscopy, UV-VIS spectroscopy, water absorption analysis, and antimicrobial tests. The positive results from these analyses indicate that the film can be used as a wound dressing in the biomedical field.

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O4. Innovative Application of Hydrogels in Drug Release Systems and 4D Printing

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Hydrogels are soft materials that have high biocompatibility and stretchability, strong adhesion and self-healing capabilities. Thanks to these properties, they have been used in biomedical applications, tissue engineering (3D Bioprinter), wearable sensors and controlled drug release systems.[1] In addition to these properties, previous studies have shown that hydrogels have cooling and moisturizing effects.[2] Therefore, their use in wound care area is promising for the future. The increasing scientific studies on hydrogels which have attract interest in recent years, will provide significant contributions, particularly in the field of biomaterials.

In classical drug treatments, since medications are taken regularly and frequently, the dose either becomes insufficient or starts to exceed the threshold value. At the same time, the medication intended to reach the diseased tissue can also harm healthy tissues and organs. Drug release systems have been developed for these reasons. Owing to particulary mentioned characteristics, hydrogels are widely used in drug release systems.[3]

Moreover, some studies show that the combination of hydrogels with some substances makes hydrogels more suitable for controlled drug release. This is because as the swelling behavior of hydrogels increases, it becomes easier to regulate the drug release rate.[4]

4D printing is the printing process that uses smart materials which respond to external stimuli by changing their shape and properties over time. By adding the time factor to 3D printing, 4D printing technology has been developed. 4D printing is an advanced manufacturing technology that enables materials to acquire dynamic properties in response to environmental factors. There are two important factors in 4D printing. These factors are Stimuli and stimulus-responsive smart materials. Smart materials are materials that have properties such as decision-making, responsiveness, shape memory, and self-healing. If these properties can be provided, 4D printing can make significant contributions to the field of tissue engineering. For instance, artificial muscles can be produced with 4D printing.[5] The use of hydrogels in 4D printing can be increased by controlling their moisture absorption. For this emerging industry; developing smart materials, printing methods, or software will support new advancements in various sectors and make life easier for many people.

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O5. Deposition rates and annealing effects on the growth of Nb thin film on Cu substrate: Molecular dynamic simulation LABLALI Mohammed ^{1*}, MES-ADI Hassane ², MAZROUI M'hammed¹

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To tackle the complexity of grasping atomic-scale structures and unraveling the factors affecting the development of thin films. In our work, we perform the deposition of Nb atoms on Cu substrates using the molecular dynamics simulation combined with the embedded atom method to describe the interaction between different atoms. We investigated the impact of varying deposition rates and thermal annealing processes on the microstructural, morphological, and mechanical characteristics of the deposited Nb film [1]. Our findings reveal that Nb atom growth on the Cu substrate occurs in island mode, accompanied by the presence of nucleation phenomena during growth. On the other hand, mixing behavior was observed at the interface between the film and the substrate, where Nb penetration is initially limited to the first Cu layer, whereas Cu atoms diffuse until reaching the third layer in the Nb film. Furthermore, Nb exhibits a BCC structure, with a significant concentration observed at a rate of 5 atoms/ps, and annealing further amplifies these percentages. Deposition at different rates leads to distinct levels of compressive normal and biaxial stress.

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O6. Development of thermoelectric composites with catalytic functionality

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The pursuit of sustainable and cleaner energy is one of the major concerns today, as energy demand has reached unprecedented levels. Every day, large amounts of waste heat generated by various processes go unutilized, leading to a loss of up to 60% of the associated energy. This untapped, low-cost thermal energy is readily available and can be recovered. Thermoelectrics have emerged as a promising green technology to convert this waste heat directly into electrical energy. This work aims to introduce a new concept that combines thermoelectric and catalytic functionalities within a single system. The concept is based on the microstructural design of thermoelements with graded porosity, which allows control over the catalytic reaction rate and the corresponding thermal effect. A key challenge is the development of efficient microstructural architectures that integrate both thermoelectric and catalytic functionalities, incorporating multifunctional elements with graded porosity into a system capable of demonstrating combined performance. In this study, a ceramic emulsification process was used to fabricate strontium titanatebased ceramics with designed porosity [1]. Using the Taguchi method, three variables with three levels were selected in the emulsification process to assess the effects of paraffin content as a pore-former, surfactant concentration, and sintering temperature. Strontium titanate was chosen as a model system, providing initial processing guidelines for obtaining porous ceramics based on this material [2]. These guidelines will further be applied to prepare novel composite materials, consisting of Pr-substituted strontium titanate as a matrix and MoNi4 intermetallic micro- and nanoparticles, which exhibit combined thermoelectric and catalytic functionalities. Preliminary results on both the processing of porous ceramics and the thermoelectric performance of these new composites will be presented.

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O7. Investigation of α-FeOOH/Dox/PEG system for controlled drug delivery

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"Drug delivery" is a term that has been used for giving or applying medicine to the human body to treat a specific disease or provide a healing effect towards a particular part of the body [1]. Generally, drugs have been used in systemic routes such as oral, intravenous, intramuscular etc. However, drug administration using systemic routes can cause some problems with drug specificity and controlling the dose of drugs. Uncontrollable drug delivery can lead to high drug doses that can cause toxicity and harm to healthy body parts [2]. To overcome these problems, studies focus on controlled drug delivery systems and mechanisms.

 α -FeOOH (goethite) is a common iron oxyhydroxide that can be found in nature. The properties of α -FeOOH, such as low cost, high specific surface area, nontoxicity and abundance, makes it an excellent material for different application areas [3]. In addition, α -FeOOH is an amphoteric material that can alter the surface charge with pH change. Altering the pH makes goethite a material that can adsorb different charged molecules. Also, α -FeOOH is a narrow-band semiconductor, which makes it absorbs visible light [4]. In this study, doxorubicin was adsorbed onto α -FeOOH and capsulated with PEG. Material characterizations and drug delivery studies were realized and discussed.

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O8. Advancements in Mechanical and Bioprosthetic Heart Valve Technologies

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Valvular heart disease (VHD) is becoming increasingly prevalent in both industrialized and developing countries, with links to congenital abnormalities and the aging population [1]. VHD accounts for approximately 20% of all cardiac surgical procedures, with more than 250,000 heart valve replacements performed annually worldwide [2]. Heart valve replacements are among the most widely used prosthetic interventions to address this condition [3]. Since the 1960s, valve replacement procedures have evolved, offering surgeons a wide range of prosthetic heart valves. These valves are primarily categorized into mechanical heart valves (MHVs) and bioprosthetic heart valves (BHVs) [4]. Mechanical valves are constructed entirely from synthetic materials, such as plastic and metal, while bioprosthetic valves are derived from animal or human tissue sources. Mechanical heart valves are crucial in the treatment of heart valve disease, providing vital support for patients requiring valve replacement. In contrast, bioprosthetic valves offer a lower risk of thrombosis compared to mechanical valves, thereby eliminating the need for long-term anticoagulation therapy. Bioprosthetic heart valves are often preferred over the more durable mechanical valves due to their reduced risk of thrombotic and bleeding complications, in addition to the benefit of avoiding lifelong anticoagulation therapy [5]. It is generally recommended that patients under the age of sixty-five receive mechanical valves due to their durability, while bioprosthetic valves are advised for patients over sixtyfive to minimize potential complications associated with anticoagulant use [6] However, structural valve degeneration (SVD), an unavoidable condition that limits the lifespan of grafts, is a common issue in BHVs [7]. SVD is marked by chronic degenerative changes in the prosthesis, including pannus formation, leaflet fibrosis and calcification, delamination of the connective tissue, and the emergence of ruptures and perforations, all signs of an irreversible process [8,9]. Both mechanical and bioprosthetic valves have been clinically used, though they often lead to complications related to anticoagulant use, immune-induced calcification, and prosthetic deterioration. For routine use in cardiovascular surgery, reliable availability of decellularized heart valves with various sizes and geometries is essential [10]. With the increasing incidence of severe VHD in adults in developing countries and the rapidly aging population in developed nations requiring life-saving procedures [10], there is a pressing need for innovative solutions to enhance the longevity and functionality of mechanical heart valves.

This study aims to comprehensively examine the advantages, disadvantages, and clinical outcomes of emerging mechanical and bioprosthetic heart valves, shedding light on their potential implications for the future of heart valve technologies.

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O9. Drug delivery study of PCL and PVP-based hydrogels with shape memory property

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Stimuli-responsive materials have been classified as smart materials. Shape memory materials are one of the smart materials, and after a shape change, they can recover their initial shape with an effect such as heat, light, pressure etc. [1,2]

This study aimed to develop a shape memory system loaded with diclofenac using polycaprolactone (PCL) and poly(vinyl pyrrolidone) (PVP)-based hydrogels and to investigate how this system affects controlled drug release.

In the study, PCL polymer with shape memory properties was homogenized by dissolving in chloroform. PVP was used to form a hydrogel, which was prepared to encapsulate diclofenac molecules. The resulting hydrogel was mixed with PCL solution, and after obtaining a homogeneous mixture, it was poured onto a flat surface to evaporate the solvent. This process resulted in a thin and homogeneous membrane. Drug release characteristics were determined by measuring them with a UV spectrophotometer.

The study revealed that PCL and PVP-based hydrogel can be used as an effective drug delivery system for shape memory polymers. These findings offer new perspectives on the use of shape memory polymers in biomedical applications.

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O10. Rehabilitation of plastic-laden soils: a preliminary study using saprophytic fungi and polyethylene terephthalate

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Agricultural soils may represent a large reservoir for plastic particles. Current agricultural practices rely on many plastic-based materials for irrigation, mulching, or greenhouse planting. Saprophytic fungi are hypothesized to be a promising cleansing strategy due to their role as natural decomposers fitting both as agriculture soil remediators while being eco-friendly. To address this topic, an experiment was conducted to assess the biodegradation potential of two saprophytic fungi, *Trametes versicolor* (Tv) and *Pleurotus sajor caju* (Psj), on a common plastic material (polyethylene terephthalate - PET). The treatments, each with 4 replicates, included Tv and Psj only, Tv+PET, Psj+PET, PET only, and the control containing solely minimal salt media. The assay was assembled in 250 mL minireactors over 56 days with sampling points at day 0, 14, 28, 42, 56. The biodegradation process was monitored by ammonia production, alkaline and acid phosphatases, pectinase, and cellulolytic activity in fungi exudates, as well as PET pellets weight and functional groups FTIR characterization.

Ammonia nitrogen production increased up to day 14 in all treatments, decreasing afterwards, except for Psj+PET. Regarding acid phosphatase, in the treatments Psj+PET and PET solely showed a tendency to increase from day 0 to day 14, while decreasing afterwards, and in treatment Psj solely it showed an increment compared to the other treatments at day 56. About alkaline phosphatase, all treatments presented a high oscillation between sampling times, decreasing from day 0 to day 14 and increasing up to day 42, except for Psj+PET. Regarding cellulolytic activity, the global tendency was an increase from the first two sampling points to the two last sampling points, although this tendency was also observed in PET solely. Pectinase activity presented a similar trend, as the activities in all treatments remained stable until day 42nd. Afterwards, at day 56, the treatments Psj, Psj+PET and Tv+PET showed a high increase in the activity of this enzyme. This trend was also observed in PET solely. Regarding the PET pellets weight, pellets of Psi+PET had a 5.72% weight loss at day 56, unlike the treatments of Tv+PET and PET solely. Regarding functional groups, FTIR spectra revealed that, regarding the peak corresponding to lipids with functional groups CH, the treatment that recorded the major area in almost all sampling days (except day 28) was Psj+PET. In the peak corresponding to polysaccharides, PET was the one recording the highest areas, except for day 28. To conclude, the reduced activity of some enzymes in the presence of PET may indicate a potential toxicity induced by the plastic. However, these fungi may have other mechanisms to persist over time and deal with plastic pollution in soils, namely cellulolytic and pectinase activity that increased in the two last sampling points. These results are further supported by the pellets weight loss, especially in treatments exposed to Psj. The *Pleurotus* genus is thus suggested to be harnessed in future studies to check for the potential degradation of other plastic polymers in soil matrices.

O11. Assessment of the potential ecotoxicity of carbon and wood fibers targeting its incorporation into new products <u>Cátia Venâncio</u>^{*}, Sara Costa, Márcio Barreto, Isabel Lopes

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Faced with increasing loads of waste generated every year, the European Union has driven a global transition towards a more sustainable, bio-based and circular economy. This transition involves, among others, investment and innovation in recycling materials to generate new products that conform with environmental sustainability. This study aimed to evaluate the ecotoxicity of eluates prepared from carbon fibers (CF) and wood fibers (WF). Eluates were prepared in a proportion of 1:10 (m:v) and tested in a dilution range from 100% to 0.59%. The battery of bioassays using key trophic level species included the producer Lemna minor (yield, growth rate, and dry weight), the primary consumer Brachionus calyciflorus (mortality), and the secondary consumer Danio rerio (mortality, hatching, larvae length). Whenever possible the lethal or sublethal dilutions causing 20% and 50% of effect [L(E)D₂₀ or L(E)D₅₀] were estimated. Preliminary data suggested that both CF and WF induced similar toxicity at the lethal level to both B. calyciflorus and D. rerio. However, at the sublethal level in D. rerio (hatching, larvae total length), WF were more toxic: the EC_{50,hatching,WF} was 17.7% and the EC_{20,length,WF} was 16.9%, while no significant effects were induced by CF in D. rerio hatching or length. For L. minor, WF induced significant effects on macrophytes' yield, growth rate, and dry weight, with estimated EC₅₀ values of 30.6%, 42.3%, and 36.4%, respectively. The integration of this ecotoxicological assessment during the development of new products that incorporate recycled materials, supports their environmental friendliness and sustainability, thus, being a key step to accelerate innovation in the recycling industry and the market introduction of more sustainable products.

O12. Heterogeneous interfaces effect on the mechanical behavior of Ag/Cu bilayers

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In this study, the nanoindentation process of a silver (Ag) coating film on a copper (Cu (111)) substrate orientation is examined utilizing molecular dynamics (MD) simulations. Three bilaver configurations of Ag namely Ag (100), Ag (110), and Ag (111) are analyzed to investigate the influence of heterogeneous interfaces on deformation behaviors. The results indicate that the Ag (111)/Cu (111) bilayer displays a greater force during the nanoindentation process in comparison to Ag (100) and Ag (110). This observation suggests that interfaces with a smaller mismatch in the specified crystal plane between Ag and Cu exhibit increased hardness. Furthermore, various indentation velocities ranging from 120 m/s to 200 m/s were considered, with indentations performed on the Ag (111)/Cu (111) bilayer. The findings reveal that variations in indentation velocity significantly affect the mechanical properties of Ag (111)/Cu (111) bilayers. Both force and hardness values demonstrate a notable increase as indentation velocity rises, indicating that the strength of Ag/Cu bilayers is more pronounced at elevated indentation velocities. These observed trends are attributed to the formation of defects and dislocations at the interface, as corroborated through dislocation extraction analysis (DXA).

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O13. Overcoming oxygen surface diffusion limitations in lanthanum nickelate Ruddlesden-Popper electrodes via praseodymium oxide infiltration for Solid Oxide Cells

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Solid Oxide Cells (SOCs) are versatile devices capable of operating reversibly, enabling either the production of electrical energy or the synthesis of valuable chemicals, such as hydrogen. Due to environmental, health, and material degradation concerns, there is increasing interest in developing cobalt- and strontium-free oxygen electrodes for SOCs. In this context, Ruddlesden-Popper (RP) phases $La_{n+1}Ni_nO_{3n+1}$ (n = 1 and 3) have emerged as promising candidates, owing to their high electrical conductivity and distinct mixed ionic-electronic properties [1]. However, these RP phases still face significant hurdles due to limitations in oxygen transport, which preferentially occurs at the surface during the oxygen reduction reaction (ORR) [2]. To improve surface kinetics, we impregnated praseodymium oxide (PrO_x) nanoparticles into the RP electrodes. Two compositions were studied: La₂NiO_{4+ δ} (L2N1) and La₄Ni₃O_{10- δ} (L4N3). The L2N1 composition exhibited superior performance, primarily due to enhanced bulk oxygen ion diffusion, thereby improving ambipolar conductivity - critical for oxygen exchange near the electrolyte. In PrOx-impregnated samples at 700 °C, the total polarisation resistance (Rpol) decreased to ~0.6 Ω cm² for L2N1+PrO_x and ~0.8 Ω cm² for L4N3+PrO_x, a reduction by a factor of ~7 and ~17, respectively, compared to non-impregnated samples. Electrochemical measurements indicate that PrO_x infiltration promotes oxygen dissociative adsorption and improves charge transfer, thereby enhancing polarisation processes. The electrochemical performance and stability of these RP phases under oxidising conditions, coupled with the oxygen transport properties and mixed oxidation states of praseodymium oxide (Pr⁴⁺/Pr³⁺), offer a promising cobalt- and strontiumfree solution for SOC oxygen electrodes.

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O14. Solution-blown spun cobalt oxide nanofibers as electrocatalysts with enhanced oxygen evolution reaction activity

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Traditional energy generation, particularly from fossil fuels, releases significant amounts of CO₂ emissions, contributing to global warming and environmental degradation. Producing hydrogen via water decomposition (water splitting) can offer a cleaner alternative by generating energy without direct carbon emissions. However, for this technology to reach its full potential, the development of stable electrocatalysts is critical. A key focus is on creating materials with enhanced selectivity for H₂ and O₂ gas formation through the Hydrogen Evolution Reaction (HER) and, mainly, in the Oxygen Evolution Reaction (OER), which is a rate-limiting step due to the occurrence of side reactions. One of the main challenges is the development of electrocatalysts with a high specific area, which would improve reaction kinetics [1]. In this context, cobalt oxide ceramic nanofibers show a great promise for potential applications in electrocatalysis and energy storage. On the other hand, the production of nanofibers from ceramic materials still faces challenges, especially in terms of production rates and solvent selection. The Solution Blow Spinning (SBS) technique has emerged as a very efficient alternative for overcoming these limitations [2]. Cobalt oxide nanofibers were produced using SBS, and the investigation was based on their structural, morphological and electrocatalytic properties in alkaline solutions (1M KOH). Calcination at 600 °C resulted in nanofibers without secondary phases, while nanofibers at 400 °C presented a phase composed of Co₃O₄-CoO. The nanofibers presented a rough morphology with monomodal distribution, and average diameter ranging from 385 nm to 485 nm. The presence of oxygen vacancies and species with higher oxidation states (Co³⁺) were beneficial in improving the OER. Calcination at 600 °C provided an overpotential (n_{10} =330 mV) more efficient Tafel kinetics and low charge transfer resistance when compared to nanofibers calcined at 400 °C. These results suggest that cobalt oxide nanofibers produced via SBS exhibit competitive electrocatalytic activity, comparable to other state-of-the-art systems, and offer new insights into the development of electrocatalysts based on structure and properties.

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O15. Synthesis and in vitro drug release of gentamicin-loaded gelatin-chitosan hydrogel

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Abstract

In this study, hybrid hydrogels containing chitosan (CS) and gelatin (GEL) were investigated. A freezing-thawing process was applied to the hydrogel prepared in equal proportions (1:1). The functional groups of the hydrogel were characterized using FT-IR spectroscopy, and the loading and release capacities of gentamicin were evaluated. The results demonstrated the successful synthesis of gentamicin-loaded CS-GEL hydrogel via the drug impregnation method and showed that controlled release occurred, indicating the potential of this hydrogel as a drug carrier.

Introduction

Three-dimensional polymeric network hydrogels can be formed with synthetic and natural polymers [1]. They can be prepared using various cross-linking methods. Physically cross-linked hydrogels may have their polymeric network structures disrupted by environmental factors. For this reason, chemical cross-linking agents are preferred [2]. Due to their soft and flexible nature, hydrogels have the ability to mimic tissues. This makes them a focal point for drug delivery and tissue engineering [1], [3]. Chitosan, biocompatible, non-toxic, biodegradable, accelerates wound healing [1]. Gelatin is biodegradable, biocompatible, and can absorb up to 5-10 times water its own weight [1], [4]. Gentamicin is an antibiotic preferred in clinical applications for treating bone infections [5]. This study aims to provide information on the synthesis of CS-GEL hydrogel and the loading and release of gentamicin through the drug impregnation method.

Method

Initially, 0.75 g of gelatin was resolved into 5 mL of distilled water (DW) by stirring on a magnetic stirrer at 40°C for 24 hours. Simultaneously, 0.15 g of chitosan was resolved

into 2% (v/v) acetic acid solution (100 µL of acetic acid + 4.9 mL of DW) via stirring on a magnetic stirrer for 24 h at room temperature. The resulting solutions were combined in a 1:1 ratio and mixed at 40°C until a homogeneous solution was obtained. Then, 0.6 mL of glycerol was added as a plasticizer to the hydrogel and mixed by a magnetic stirrer for 20 minutes. Tannic acid, as a crosslinking agent, was added to the CS-GEL solution at 2% by weight of the total polymer and mixed by a magnetic stirrer at 40°C for 24 h. The prepared solution was transferred into a petri dish and left at room conditions for one night to remove air bubbles. The hydrogel was subjected to a freezing-thawing process, including freezing at -20°C for 20 h and thawing for 4 h, in 3 cycles. Gentamicin was added to the hydrogel using the impregnation method, and a drug release study was conducted. The loading and release of gentamicin were evaluated using UV-Vis spectroscopy. Finally, the functional groups of the hydrogel were characterized using FT-IR spectroscopy.

Results

In the prepared CS-GEL hydrogel, plant-derived polyphenol tannic acid was used as a crosslinker. According to the FT-IR results, all synthesis steps were successfully completed, and according to the *in vitro* drug release results performed for the hydrogel, the drug release of gentamicin was successfully achieved.

Discussion

In a PBS solution simulating the body environment, it was observed that the *in vitro* release of gentamicin occurred in a controlled manner, demonstrating the potential of this hydrogel for controlled drug delivery systems.

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O16. The Process of GaN-on-Diamond with Si Nano-intermediate Layer SAB Technology

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Gallium nitride (GaN) high electron mobility transistor (HEMT) structures have shown great application in many radio frequency applications, such as 5G Wireless Communication Technologies, and high-power devices due its ability to produce 2-dimensional electron gas (2DEG). Building on silicon electronics technologies, GaN is often grown on Si/SiC wafers to allow for efficient manufacture using well established device process and tooling. Current GaNon-Si devices suffer from poor thermal transport, reducing the effectiveness of the device due to the thermal transport limitations [1]. There is a large drive to utilise the higher thermal conductive materials to help dissipate the excess heat to increase the efficiency of the device.

Here, we utilise Diamond, which has thermal transport coefficients up to 4 times that of Si/SiC, with up to 2000 W/mK. 10-100 devices could be fabricated on the transparent 1-inch GaNon-Si wafer. The liquid metal gallium alloys key technology of no seed crystal or added pressure was raised by Ruoff's team in 2022, only diamond particles were found [2]. But there are still many technical barriers of GaN growth for CVD equipment. We propose an improved diamond thin-film synthesis method of based-Ga liquid metal on silicon substrate, and assemble the GaNon-Si and Diamond-on-Si wafers by surface Ar-ion active bonding [3]. 1-inch GaN-on-Diamond wafer for the diamond thin-film thickness of 100 μ m were performed, and an amorphous Si intermediate layer of 10 nm was formed at the bonding interface, which played a critical stress release role and transformed heat dissipation into diamond substrate with small observable thermal boundary resistance.

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O17. Prospects for electrodeposition of iron from mixed magnetite-metallic iron suspensions for steel production

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The use of iron-containing wastes and residues as feedstock for iron production is seen as a key advancement in enhancing sustainability and contributing to the circular economy [1,2]. However, impurities in the iron oxide feedstock introduce significant challenges during the electrowinning process for green steelmaking, leading to unpredictable effects. In the present study and, for the first time, the impact of metallic iron content on the Faradaic efficiency and microstructure of the obtained iron deposits was evaluated through the electroreduction of iron-magnetite powders in alkaline suspensions (10 M NaOH) at low temperature (80 °C). Samples with varying magnetite/iron ratios and a fixed magnetite content, both with and without the presence of iron, were prepared and characterised. The characterisation included combined SEM/EDS/XRD analyses. particle size distribution. cvclic voltammetry and chronoamperometry studies. The results reveal that the presence of metallic iron may negatively impact the reduction process. A comparative analysis of suspensions with and without iron content showed that the Faradaic efficiency for iron-free samples (63-76%) significantly exceeds that for iron-containing suspensions (37-57%). This demonstrates that the presence of metallic iron in the suspension can hinder the electroreduction of magnetite to metallic iron, with the effect becoming more pronounced at higher Fe concentrations. Changes were observed in the microstructure of iron deposits, with the dendrites becoming less sharp and more disordered in iron-containing suspensions. Particle size distribution analysis further revealed that larger metallic iron particles may contribute to the sedimentation and entrapment of magnetite particles, which negatively affect the current density and Faradaic efficiency.

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O18. Investigation of local properties and corrosion of copper and mild steel with different surface morphology

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Corrosion is a natural process that occurs when metal is exposed to certain environments or substances. The effects of corrosion can be devastating in industrial settings, leading to costly downtime, repairs, and lost productivity - not to mention potential risks to life and limb if left unchecked. Awareness of corrosion prevention and control is essential to ensure the smooth and safe operation of any process. Corrosion 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. Corrosion is therefore a subject of interest to interdisciplinary research, combining fields of materials science, chemistry, physics, metallurgy and chemical engineering. For understanding of these material science phenomenon, powerful microscopy tools are of utmost importance as they provide detailed insights into the intricate nature of material at micro scales. It is necessary to know how the local morphology of the surface (local dents, defects, scratches) affects their physical properties of the surface. These defects are of a local nature and to study the influence of these defects it is also necessary to use local methods. The methods of AFM (atomic force microscopy), nanoindentation, microscratching are successfully used to study the physical properties of materials.

In this work we investigated local properties during corrosion in distilled water of mild steel copper by AFM methods after local mechanical deformation (micro-scratching, polishing). According to Kelvin probe force microscopy (KPFM), the surface potential changed in the deformed region after deformation, and the additional modulation of the surface potential corresponded to the local shape of the surface (bending). Correlations during corrosion, surface potential 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.

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O19. Synthesis and Characterization of Ag/Ag₃VO₄@rGO Nanocomposite Photocatalysts for Photocatalytic Food Dye Degradation <u>Esra ÇAKAR^{1,2,*}</u>, Mahmut ÖZACAR^{2,3}

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- Abstract

The aim of this study is to combine Ag/Ag₃VO₄ with rGO using a hydrothermal technique to form nano-composites. During the hydrothermal process, the composite materials at various concentrations were fabricated at the optimum synthesis conditions, and characterized via different techniques. Then, these prepared nanocomposite structures were utilized to remove food dyes in various waters.

- Introduction

In recent years, the use of dyes has proliferated in a multitude of industrial sectors, including textiles, leather, metals and food, due to the rapid growth of the global population and the significant role that dyes play in enhancing the quality of life of individuals. While dyes enhance the visual appeal and opulence of our lives, they also give rise to certain environmental concerns. As evidenced by research, the annual release of dyes into waterways amounts to over seven million tons, resulting in the generation of wastewater containing these substances. The release of dyed wastewater represents a significant threat to the protection and development of the natural environment. Furthermore, the wastewater resulting from the dyeing process contains a variety of hazardous heavy metal components and organic compounds that impair water clarity, cause significant visual pollution and contribute to the destruction of aquatic habitats. The existence of dyes in wastewater causes a significant threat to the habitats of humans and aquatic organisms. In comparison to clean water, dyed wastewater is characterized by darker colours, higher acidity and a higher biological and chemical oxygen demand. To address the issues associated with dyed wastewater, experts have proposed a range of strategies, including adsorption, flocculation, and coagulation. Nevertheless, it is challenging to implement effective solutions for the removal of dye wastewater. The possibility of producing numerous intermediate compounds with enhanced stability and elevated toxicity during the purification process may result in a higher purification cost. Consequently, a significant number of scientists have concentrated their efforts on the development of innovative technologies to address these challenges [2].

- Method

Synthesis and characterization of Ag/Ag₃VO₄ nanostructures

A solution of 0.3 g ammonium metavanadate (NH₄VO₃) in 20 mL ultrapure water was prepared. The mixture was then homogenized in a magnetic stirrer for a period of 30 minutes. Subsequently, 0.3 g of silver nitrate (AgNO₃) was dissolved in 20 mL of pure water in a separate beaker and homogenized in a magnetic stirrer for 30 minutes. The aforementioned mixtures were then transferred to a Teflon-based autoclave and subjected to a heat treatment at 180 °C for 24 hours. The Ag/AgVO₃ nanostructures were washed three times with pure water and once with methanol, after which they were subjected to centrifugation in order to remove any residual impurities. The characterization of the synthesized Ag/AgVO₃ nanostructures was conducted through the utilization of XRD and SEM techniques.

Synthesis and characterization of rGO nanostructures

The Hummers method was employed in the synthesis of rGO. A solution of 16 mL concentrated H_2SO_4 was added to a mixture of 10 g graphite and 5 g P_2O_5 . Subsequently, 6 g $K_2S_2O_4$ was added and the solution was refluxed at 80°C for a period of 2 hours. Subsequently, the solution was cooled to room temperature and allowed to stand overnight in the dark. The solution was then washed several times with pure water until the pH is neutralized. In order to complete the oxidation of this partially oxidized graphite, 34 g of KMnO₄ and 240 mL of H_2SO_4 solutions will be slowly added in an ice bath at 0 °C. The temperature of the mixture was monitored and maintained at a constant level to ensure that it does not exceed 20 °C. Subsequently, 1 L of pure water was added to the aforementioned mixture and refluxed at 35 °C for a period of 2 hours. Subsequently, 20 mL of H_2O_2 was added to the solution, thereby initiating the reduction process. Subsequently, the mixture was subjected to a washing process with a 1:10 HCl solution (1 L) in order to remove any residual metals and impurities. Subsequently, the dark brown rGO nanoparticles was subjected to an oven-drying process for a period of 12 hours. The characterization of rGO was carried out by Raman technique.

Photocatalytic degradation study

Photocatalytic activities of the developed nano photocatalysts were investigated by dye degradation under UV and visible irradiation. In each experiment, 50 mg of photocatalyst was added to 250 mL of 16 ppm dye aqueous solution. Before exposure to UV and visible irradiation, the suspensions were stirred with a magnetic stirrer in the dark for 30 minutes to ensure the adsorption-desorption balance of the dye on the photocatalyst surface. At certain time intervals, 5 mL of the solutions were taken, centrifuged and analyzed with a UV-Vis spectrophotometer.

- Results

XRD spectrum of Ag/Ag₃VO₄ samples synthesized by hydrothermal method are given in Figure 1. It can be observed that the Ag/Ag₃VO₄ structure contains impurities in the form of tetragonal Ag₃VO₄ (ICSD: 98-041-7470) and cubic Ag (ICSD: 98-060-4635). Ag/Ag₃VO₄ nanoparticles have hexagonal unit cell and unit cell parameters a, c, V and space group are 4.997 Å, 9.69 Å, 241.98 Å³, I-42m, respectively.

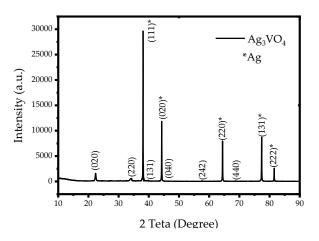


Fig. 1. The XRD pattern of Ag/Ag₃VO₄.

FE-SEM images of Ag/Ag₃VO₄.

SEM surface images of Ag/Ag_3VO_4 samples synthesized by the hydrothermal method are given in Figure 2. When FE-SEM images are perused, it is seen that the samples' particle sizes are in the 30-100 nm range. It was observed that there was no impurity in the XRD and FE-SEM results. However, it is seen that Ag and Ag_3VO_4 forms are together in the AgVO4 structure.

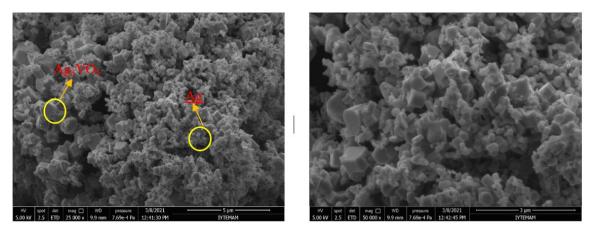


Fig 2. FE-SEM images of Ag/Ag_3VO_4 .

- Discussion

The present study concerns photocatalytic dye degradation by rGO and Ag/Ag_3VO_4 composite photocatalysts. In this study, rGO and Ag/Ag_3VO_4 nanoparticles were synthesized by the hydrothermal method. The photocatalytical effect was analyzed through a UV-Vis spectrophotometer. It was observed that photocatalytic degradation of food dyes via the prepared composite photocatalysts increased by 10% compared to pristine rGO and Ag/Ag_3VO_4 .

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O20. Development of a novel efficient Ni-CeO₂-Gr ternary nanocomposite coatings for Enhanced Corrosion and Wear Resistance

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In this study, a novel Ni-CeO₂-Gr nanocomposite coating was developed on a Cu substrate through electrochemical co-deposition in a conventional Watts bath. Graphene (Gr) nanosheets were synthetized via electrochemical exfoliation. pure Ni, Ni-Gr, Ni-CeO₂, and the ternary Ni-CeO₂-Gr were characterized using optical microscopy, scanning electron microscopy (SEM) with energy-dispersive spectrometry (EDS), X-ray diffraction (XRD), Raman spectroscopy, Vickers microhardness, and micro-scratch testing. Electrochemical properties were assessed via electrochemical impedance spectroscopy (EIS) and DC-polarization in 0.5 M NaCl. SEM-EDS, Raman, and XRD analyses confirmed the successful synthesis of graphene and the integration of CeO₂ nanoparticles and graphene nanosheets within the nickel matrix. The ternary Ni-CeO₂-Gr coating demonstrated superior microhardness (915.6 HV), cohesive strength, and enhanced corrosion resistance (544 K Ω .cm²) compared to pure Ni coatings (30 K Ω .cm²), attributed to the synergistic interaction of graphene and CeO₂ layers within the Ni matrix, which forms a resilient anticorrosion barrier. These insights contribute to the development of high-performance materials for corrosion protection in challenging environments.



O21. Copper-based films obtained by anodization for supercapacitor applications

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The field of renewable energy is rapidly growing, exemplified by the European Union's Green Deal, which aims to make the EU the first climate-neutral region in the world by 2050. While renewable energy offers many benefits, it also presents challenges, particularly because its energy production is not continuous. This highlights the need for more cost-effective energy storage solutions/devices with high capacitance.

One of the solutions would be the employment of supercapacitors. They are long-lasting and offer fast charging/discharging. Many materials have been researched but most of them are not readily available or their manufacturing process is complicated. Copper on the other hand can offer sustainable and innovative solutions. It is a relatively abundant and cheap metal, and its hydroxide has high specific capacitance [1], while theoretical capacitance of oxides can reach even higher values: $Cu_2O - 2247.6$ F/g [2], CuO - 1783 F/g [3].

Copper foil and foam electrodes were used in our study. Cu(OH)₂, Cu₂O and CuO films were obtained in NaOH solution by applying cyclic voltammetry dependently on the potential. In Na₂CO₃ solution the formed films was containing mostly Cu₂O and some CuCO₃. The surface morphology, chemical composition and the phase composition were evaluated by SEM, EDS and XRD, respectively.

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O22. The application of nanomaterials as the vaccine carrier in fish

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Vaccination as an effective measure to prevent and control fish diseases, has been valued and adopted by many countries. Among the various immunization methods, immersion vaccination has the advantages of saving time and effort, and being less irritating to the fish and widely used in aquaculture. However, due to the biological barrier of fish skin, vaccines are difficult to enter into the body and significantly reduce the immune effect, which is the bottleneck of immersion vaccination. The nanocarrier strategy is one of the effective measures to figure out this issue. Nanomaterials including carbon nanotubes (CNT) and bacterial nanocellulose (BNC), which has been proved to possess outstanding properties such as excellent permeability, stiffness, low density, biocompatibility, and renewability, have huge potential serving as the delivery carrier for the design of novel drugs, proteins and vaccines. Streptococcosis is a highly contagious aquatic bacterial disease that poses a significant threat to tilapia, which is the second-largest farmed fish after carp and one of the fish widely cultured around the world. Streptococcus agalactiae (S. agalactiae) and Streptococcus iniae (S. iniae), the two main pathogens of tilapia streptococcosis.

In this study, the surface immunogenic protein (Sip) and Enolase (Eno) were identified to be conserved and hold potential to provide cross-immunoprotection for both S. agalactiae and S. iniae by multiple sequences alignment and Western blotting analysis. On this basis, we expressed and obtained the recombinant protein rSip and rEno, and connected them with functionalized CNT and BNC to construct the nanocarrier vaccine systems CNT-protein and BNC-protein. After immersion immunization, the immune effect of nanocarrier vaccine systems against two streptococcus infections was evaluated in tilapia based on some aspects including the serum specific antibody level, non-specific enzyme activities, immune-related genes expression and relative percent survival (RPS) after bacteria challenge. The results showed that compared with control group, nanocarrier vaccines significantly (P < 0.05) increased the serum antibody levels, related enzyme activities including acid phosphatase, alkaline phosphatase, lysozyme and total antioxidant capacity activities, as well as the expression levels of immunerelated genes Besides, the above indexes of nanocarrier vaccine groups were higher than those of pure protein groups with different extend during the experiment. Furthermore, the challenge test indicated that nanocarrier vaccines provided cross-immunoprotection against S. agalactiae and S. iniae infection, respectively, which were much higher than those of other groups. Our study indicated that the nanocarrier vaccine CNT-protein and BNC-protein could induce protective immunity for tilapia through immersion immunization and may be an ideal candidate vaccine to prevent and control tilapia streptococcal disease, which also provided a significant reference for the controlling of fish diseases in aquaculture.

O23. Atomic layer deposition of TiO₂ thin films - enhanced tool for photocatalysis

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Rapid urbanization and industrialization threaten environmental safety and the health of the community. Photocatalysis is a promising process that harnesses abundant solar energy for water purification, presenting a green approach to environmental management. Semiconductor metal oxide, particularly titanium dioxide (TiO₂), is commonly used as a photocatalyst due to its excellent physical and chemical stability and environmental friendliness. However, the main lack in semiconductor-based photocatalytic processes is the fast recombination of the photogenerated electron-hole pairs [1], which reduces efficiency.

Atomic layer deposition (ALD) is an advanced synthesis technique that allows control over catalyst design, including morphology and active sites at the atomic level. A recent study demonstrates that the grain size of an anatase TiO₂ film can be tailored and controlled on different substrates not only by the processing temperature and film thickness, but by the nanometric intermediate Al₂O₃ layer deposited on substrates in the same ALD sequence [2]. Another study demonstrates the influence of grain size on the photocatalytic activity of TiO₂ thin films grown by ALD technique. Thin films with different crystalline structures and grain sizes were grown on silicon substrates under different synthesis conditions, by changing the reactor temperature, deposition time or intermediate layers. The photocatalytic activity was assessed by measuring methylene blue (MB) degradation rates in aqueous solutions under ultraviolet irradiation. The results indicated that grain size significantly affects MB degradation [3].

While TiO_2 is an effective photocatalyst, its efficiency in removing organic compounds in wastewater under solar light is limited, as only about 3–5% of solar light is in the ultraviolet (UV) range, while nearly 45% is in the visible spectrum [1]. Consequently, a significant challenge is to develop green and sustainable thin-film materials that can make full use of solar irradiation for practical applications. One approach to overcome these limitations is to dope TiO_2 with various alkali, transition, noble, or rare-earth metals, as well as non-metal elements such as nitrogen (N), carbon (C), sulfur (S), and iodine (I). Doping TiO_2 in this way can narrow its band gap, enabling it to absorb more visible light and enhancing its photocatalytic efficiency under solar irradiation.

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O24. An effective sealing method for planar solid oxide fuel cells using compressed vermiculite

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Population growth has led to a constant increase in global energy demand [1], and facing their energy necessity without contributing to climate change has set the scientific community to explore clean and effective power delivery technologies [1]. A nearby commercialization candidate from the existing technologies to efficiently produce electricity are the fuel cells [2], specifically solid oxide fuel cells (SOFC) - high-temperature fuel cells that present several benefits as the fuel flexibility for the electrochemical reaction. However, one of the main drawbacks that are limiting the technology development is the sealing of devices, typically made by using glass-seal materials – a very time-consuming and ineffective way to seal SOFC.

This work aims to address this problem by developing an efficient method for sealing. A high-temperature planar single-cell was designed to advance SOFC development at the laboratory level. The cell was created to be cost-effective and provide easy and fast sealing; it was intended as an AISI316 stainless steel reactor to be sealed with a compressive material - vermiculite sheets (specifically vermiculite). The sealing approach includes the application of low compressive loadings (0.2 N m) in the cell assembly. The ex-situ and in-situ experiments showed significant results; leaks through the cell to the environment were evaluated to be only 0.4 mL min⁻¹ m⁻¹, and the electrochemical tests, made at 650 °C, revealed a high stable open circuit potential of ca. 1.04 V (with hydrogen in anode and oxygen in cathode), indicative of minimal gas crossover between cathode and anode. The cell design reliability was confirmed during the heating cycle and throughout the shutdown simulation experiment, where the cell was held successively under open circuit voltage and 0.7 V during a total period of 109 h). Results showed that the open circuit potential value was highly stable during the experiment, and the cell's performance for energy production decreased slightly from 0.16 to 0.14 A cm⁻², showing minor degradation in the studied period.

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O25. Production and Characterization of 4D Biomaterials for Drug Release

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4D (4-Dimensional) biomaterials can be triggered and activated in response to biological cues or environmental stimuli, facilitating temporal and spatial controllability of the drug programmed and loaded into the material. Stimuli can be physical or chemical, such as light, temperature, pressure, humidity, pH, magnetic/electric field, and biological stimuli. 4D biomaterials have the ability to transform and change shape in response to these stimuli in their environment. Transformational properties include self-repair, shape memory, and multifunctionality [1].

Drug delivery systems aim to deliver medicinal compounds by drug release at targeted sites. Here, drug delivery systems prepared with 4D materials are preferred to regulate drug profiles by modulating distribution, absorption, elimination, and metabolism to maximize drug performance while minimizing side effects, unlike conventional drug delivery methods that release drugs instantly [2]. Drug delivery systems require design optimization to ensure optimal performance in terms of drug release. 3D biomaterials can mimic excellent physiological properties, but biomedical materials/devices produced with this technology are inherently static and not designed for dynamic situations. 4D biomaterials, on the other hand, enable the production of more comprehensive drug delivery systems compatible with dynamic environments. 4D materials are synthesized according to their response to external stimuli and develop a deformation mechanism. This mechanism releases the drug at the desired time and place, enabling more effective and faster delivery to the targeted area [3].

Drug delivery systems prepared using 4D materials are essential for the pharmaceutical and biomedical industry and offer significant opportunities. A new era has been initiated in drug delivery systems by controlling the pharmaco-kinetics and pharmaco-dynamics of drugs with 4D materials. However, this study area is still evolving, and extensive studies are needed to understand the transformative potential of 4D materials better. Further research will contribute to the literature to better understand the mechanics and kinetics involved in these complex drug delivery systems. In this study, drug delivery systems involving 4D biomaterials have been reviewed and compared.

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O26. Innovative Skin Ageing Solution: Lipid Nanoparticles for Hyaluronic Acid Production

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Hyaluronic acid (HA) is crucial for skin health, assisting nutrient exchange and maintaining moisture [1], which supports skin elasticity and helps combat ageing [2]. This study aimed to enhance HA production in skin cells using solid lipid nanoparticles (SLNs) carrying β-carotene, a compound promoting antioxidant and anti-ageing effects [3].

β-carotene-loaded SLNs were prepared using Glycerol Monostearate (Imwitor 900K) and cacao butter with a surfactant. The SLNs were characterized for stability, particle size, zeta potential, encapsulation efficiency, and loading capacity. In vitro assays on human dermal fibroblasts and HaCaT cells evaluated by metabolical activity and HA production, measured via AlphaLISA.

The optimized β -carotene-loaded SLNs displayed high stability and encapsulation efficiency. In vitro studies demonstrated a significant increase in HA production in both fibroblasts and HaCaT cells treated with the SLNs, suggesting effective stimulation of HA synthesis.

The β -carotene-loaded SLNs effectively enhance HA production in skin cells, presenting a promising and innovative approach for anti-ageing skincare solutions.

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O27. Flexible Solid-State Supercapacitors and Organic Ion Hydrogel Sensors for Self-Powered Smart Sensing Applications

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Purpose: A self-supplied sensing system was developed by integrating flexible highperformance solid-state supercapacitors and organic ionic hydrogel sensors, which can detect physiological signals stably and continuously without an external power source, for wearable electronics as a key technology for next-generation flexible electronic devices.

Methods: Zn-Co MOFs@MXene were synthesized by top-down self-assembly of positively charged cobalt ions and zinc ions onto electronegative functional groups on the surface of MXene via electrostatic interactions, and the three-dimensional porous and flexible hydrogels were prepared by using free radical polymerization and salt precipitation effects. the salt-generated salting-out effect is utilized to enhance the electrostatic interactions, thereby improving the toughness of the hydrogels.

Results: The supercapacitor demonstrates a high energy density of 51 Wh/kg at a power density of 1.59 kW/kg. In particular, it maintains exceptional mechanical flexibility under different bending environments. The resistance change rate of the organic ionic hydrogel sensor exhibits a linear response within the strain range of 0-400% and 400-600%, respectively, and it shows outstanding electromechanical stability Furthermore, the system can be conveniently used for real-time detection of human motion and small strains.

Conclusions: We have successfully developed a self-powered integrated system consisting of flexible solid-state Zn-Co MOFs@MXene supercapacitors and PAM-BTO/NaCl organic ion hydrogel sensors. The system can be easily attached to a flexible substrate on human skin and realize functions such as real-time monitoring and testing through human-machine interaction.

O28. Minute-level Preparation as Ni(OH)₂/NiS Hollow nanorods Heterostructure for Hydrogen Evolution Reaction in Alkaline <u>Rui-dong Shi</u>¹, Jin-ju Chen^{2,*}

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Purpose: Anion-exchange membrane water electrolysis (AEMWE) system is now the most promising solution for hydrogen production, with the development of low-cost, high-performance bifunctional catalysts for hydrogen evolution reaction (HER) being the key to their commercialization.

Methods: Rapid in-situ growth of hollow rod-like Ni(OH)₂/NiS heterostructure on Ni foam (Ni(OH)₂/NiS/NF-HR) by electrodeposition and sacrificial template methods. Specifically, the one, the ZnO template is grown on nickel by a hydrothermal method. Then, ZnO/NF is electroplated in a solution containing NiSO₄, Fe₂(SO₄)₃, and thiourea, and finally, (Ni(OH)₂/NiS/NF-HR) is obtained by alkaline etching.

Results: The Ni(OH)₂/NiS/NF-HR provides more reactive sites, and facilitates the adsorption of H2O and optimizes HER (Volmer step, adsorbing H*). As a consequence, a low overpotential of 66.4 mV to achieve 10 mA cm⁻², and exhibited a high H2 generation of 105.7 s⁻¹ in alkaline solution for HER were acquired on Ni(OH)₂/NiS/NF-HR, outperforming the Ni(OH)₂/NiS/NF electrocatalysts. Remarkably, an electrolytic cell assembled by using Ni(OH)₂/NiS/NF-HR as both anode and cathode delivered an overall water splitting (OWS) current density of 10 mA cm⁻² at 1.59 V.

Conclusions: In conclusion, we have in situ grown Ni(OH)2/NiS with a hollow structure on NF by electrodeposition and sacrificial template methods, which has excellent mass transfer kinetics and greatly accelerates the HER process. This report will hopefully be used in AEMWE system, and their providing insights about the design of bifunctional catalyst.

O29. Bacterial cellulose reinforced mechanical robustness and self-repairable polyurethane composites with dual-dynamic bonds <u>Tao Cheng</u>¹, Jin-ju Chen^{2,*}

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Purpose: Incorporating dynamic bonds in polyurethanes enhances self-healing, whereas rapid network rearrangements usually sacrifice mechanical properties. The development of polyurethane materials with simultaneously fast self-repairable and mechanical robustness is still a huge challenge.

Methods: A straightforward strategy to fabricate self-repairable yet mechanically robust cellulose-based polyurethane (SCPUs) nanocomposites were present. Specifically, a disulfide crosslinker was first introduced to polyurethane backbone to form a prepolymer. Then, the SCPU nanocomposites with a dual dynamic network of abundant S-S and H-bonds were prepared through a one-pot reaction of prepolymers with bacterial cellulose nanofibers containing different contents.

Results: The H-bond interactions formed by the polyurethane carbonyl group (C=O) and the cellulose hydroxyl group (-OH) result in significantly enhance the mechanically robust of the SCPUs. As the cellulose content is increased, the tensile strength reaches 24 MPa. Moreover, The SCPUs also demonstrated excellent self-repairable capability due to the synergistic effect of the rapid exchange of dual-dynamic bonds and the entropic elasticity. The mechanical strength healing efficiency of the fractured composites without external force within 9 hours was as high as 90%.

Conclusions: In conclusion, we prepared SCPUs nanocomposites with high mechanically toughness, high elastic recovery, and high self-healing capability by introducing cellulose nanofibers into polyurethane containing dual-dynamic bonds. This work would inspire the fabrication of polyurethane nanocomposites combining mild-condition self-repairability and excellent mechanical performance.

O30. De Novo Design of Modular Click-Peptide Chimeras for Immune Checkpoint Proteins Degradation Yu-Ying Shi, <u>Meng-Yuan Dai</u>*

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Drug development is a demanding endeavor, requiring substantial resources to identify effective compounds for a limited number of targets. Targeted Protein Degradation (TPD) hold promise for addressing challenging 'untargetable' proteins but face difficulties with membrane proteins. Here we developed an exceptionally stable peptide chimera degradation platform, distinguished by its modular and streamlined design, which facilitates the comprehensive utilization of protein-protein interactions. We tested this platform by focusing on targeting the intracellular segments of challenging-to-address immune checkpoint proteins and attempting to degrade these proteins. Through a computation-guided approach, high-affinity peptide sequences for target proteins (POIs) were designed de novo, followed by multiple levels of stability modifications and optimizations. This approach revealed a correlation between peptide structure stability and enhanced degradation efficacy within the platform technology. In this theoretical framework, a type of click peptide with hyper-stable cyclic structures, created using Cu(I)catalyzed azide-alkyne click chemistry and linked to lysine side chains with high-efficiency E3 ligands, showed remarkable potency. When targeting PD-1, this clicked peptide targeting chimera (CPeTAC) exhibited a DC50 only 1/37,328th that of the basic linear peptide. Moreover, CPeTAC minimizes structural dependence, particularly in TIGIT targeting. The highly stable peptide degradation agent, created through click chemistry, has shown exceptional in vivo pharmacokinetics. This allows inherently susceptible peptides to pre-systemic enzymatic digestion to achieve favorable oral efficacy, paving the way for more efficient and convenient immune checkpoint drug development in the future. In summary, the CPeTAC technology simplifies and improves drug design, potentially leading to more efficient synthesis of drugs targeting a wide range of targets. Meanwhile, we look forward to the combination of the CPeTAC with advanced nanomaterials to achieve high-efficiency delivery of the CPeTAC, better targeting dose and drug controlled release, consequently providing new solutions for clinical anti-tumor treatment.

O31. Characteristic nanostructure and its role in ductile and fatigue failure of metallic materials Xiangnan Pan^{*}, Youshi Hong

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- Material failure typically initiates locally, such as void formation in ductile fracture or crack origins in fatigue failure. Both of these phenomena are associated with unique micro- and nano-structural features.

- Advanced material characterization techniques, e.g. focused ion beam (FIB), ion cross section polishing, electron backscatter diffraction (EBSD), transmission Kikuchi diffraction (TKD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM), are applied to the dimple ridge of ductile fractures and the crack initiation regions of high-cycle fatigue (HCF) and very-high-cycle fatigue (VHCF, failure cycle $N_f > 10^7$).

- Nanograins prevail at the ridge tips and beneath both fracture surfaces within the crack initiation regions of titanium alloys and aluminium alloys produced by conventional and additive manufacturing subjected to monotonic tension and VHCF loading, which contribute significantly to damage accumulation due to a type and a variant of severe plastic deformation (SPD).

Workshop 1.



3rd Workshop on New Challenges of Bionanomaterials: Science, Technology, Application

> University of Aveiro, Portugal, 19 November, 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.

3rd Workshop New Challenges of Bionanomaterials: Science, Technology, Application, University of Aveiro, Portugal, November 19, 2024 (WNCBM-2024)

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Bio-nanofabrication Nanostructured Materials Nanoassemblies / Surfaces **Modelling of Bionanomaterials Bio-Inspired nanomaterials Bio-nano measurement and microscopy** Nanobioanalysis in vitro Nanotoxicology Nanotechnology safety Nanomaterials for Medicine and Medical Diagnostics **Body Implants and Prosthesis Stem Cell Regeneration Tissue Engineering and Organ Transplantation Nanosurfaces and Interactions 3D** Printing of biomaterials **DNA** nanotechnology Nanotechnology for Vaccines Pharmaceutical Nanotechnology

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University of Aveiro, Portugal, 19 November 2024	
14:00– 14:20	Dr. Gil Gonçalves Pioneering New Frontiers in biomedicine with Carbon-Based Nanomaterials Centre for Mechanical Technology and Automation (TEMA)-University of Aveiro, Portugal
14:20– 14:45	Dr. Igor Bdikin Atomic Force Microscopy Methods for Characterization of Organic Materials Centre for Mechanical Technology and Automation (TEMA)-University of Aveiro, Portugal
14:45– 14:55	Duarte Almeida Microfluidic production of multifunctional nanocomposites for lithium-based neutron capture therapy TEMA – Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro

3rd Workshop New Challenges of Bionanomaterials: Science, Technology, Application 19 November 2024, University of Aveiro, Portugal

Pioneering New Frontiers in biomedicine with Carbon-Based Nanomaterials

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Carbon-based nanomaterials have unlocked new possibilities for developing advanced smart materials to address a variety of societal challenges. Progress in innovative synthetic techniques has enabled the creation of functional carbon nanomaterials with wide-ranging applications, from environmental sustainability to healthcare. Recent advances in unconventional nanoengineering methods have particularly emphasized the potential of carbon nanocapsules (CNCs) as highly effective nanomedicines, especially for cancer treatment.

CNCs (Carbon Nanocapsules) represent a groundbreaking therapeutic innovation, utilizing hermetically sealed short carbon nanotubes to encapsulate specialized payloads for cancer therapy and bioimaging. These "carbon shelters" enable the precise and safe delivery of substances that might otherwise be too toxic or inefficient for targeted applications.[1, 2] However, the toxicological risks associated with CNTs have limited their use to more invasive treatments.[3] Recent advancements include the exploration of carbon nanohorns as CNCs, demonstrating the feasibility of lithium encapsulation for neutron cancer therapy. Similarly, carbon dots have emerged as a promising alternative, capable of housing atomically dispersed gold—a significant step forward in cancer nanotheranostics. Studies indicate that imaging-guided injection of these innovative nanocapsules can suppress tumor growth in carcinoma models by enhancing mitochondrial oxidative stress, all while minimizing adverse side effects.

This work aims to explore novel strategies for developing advanced carbon-based nanomaterials tailored for cancer therapy and diagnosis. Additionally, it highlights approaches to functionalize their external surfaces with organic molecules to enhance their biological performance. These enhancements are anticipated to extend blood circulation times and improve tumor site accumulation, thereby significantly advancing the therapeutic and diagnostic effectiveness of these advanced nanoplatforms in cancer-related applications.

Acknowledgments

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Atomic Force Microscopy Methods for Characterization of Organic Materials

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In the past 20 years, various types of organic nanostructures have been found: nanotubes, nanoballs, nanorods, nanosheets. Due abnormal 2D- and 3D-shape of these materials demonstrated unique physical properties. It can be used in important applications: sensors, gernerators etc. Currently, it is becoming increasingly obvious that develop new methods for investigation of biological microstructures is extremely necessary. So, in case of virus infections (Pandemia COVID-19) one of main problem is rapid diagnosis in resource-limited settings, which are especially relevant for all global health problems of the modern world. Therefore, methods for detection, visualization, analysis of the organic microstructures must be in priority nanotechnology. One of this very perspective method is atomic force microscopy (AFM). The advent of AFM provides a potent tool for investigating the structures and properties of biological samples at the micro/nanoscale under near-physiological conditions, which promotes the studies of single-cell behaviours from one side and high resolution single organic molecules from another side. AFM has achieved great success in single-cell observation, single DNA molecules, organic microsctructures and manipulation for biomedical applications, demonstrating the excellent capabilities of AFM in addressing biological issues at the single-macromolecular level with unprecedented spatiotemporal resolution.

For effective commercial devise there several parameters: technological problems and cost, bio and ecology acceptability, value used for the practical application of the effect. Here we show the applicability and current problems of piezoresponse force microscopy (PFM) for studying a broad range of polar materials at the nanoscale for biological / organic complex materials: organic polymers, organic nano tubes, amino acids/ nucleobase, organic fibers, organic composite films, organic single crystals.

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.



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Microfluidic production of multifunctional nanocomposites for lithium-based neutron capture therapy

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Traditional cancer treatments have generally lacked sufficient effectiveness and specificity, often leading to adverse side effects, extra discomfort, and increased costs for patients [1]. Neutron capture therapy (NCT) provides an alternative approach by introducing stable isotopes, commonly ¹⁰B, into cancer cells. Once accumulated in the cells, these isotopes are exposed to a low-energy neutron beam, which, upon capture, releases short-range radiation that precisely targets and damages cancer cells with minimal impact on nearby healthy tissue. The ¹⁰B isotope, in particular, has shown substantial effectiveness in NCT applications [2]. However, these traditional boron-based compounds frequently lack sufficient biocompatibility and targeting efficiency for clinical uses, Nonetheless, the limitations in efficacy have spurred research into alternative elements such as lithium [3]. CDs not only exhibit strong biocompatibility but also possess exceptional optical properties useful for bioimaging applications. However, their extremely small size (<10 nm) can limit their delivery efficiency due to rapid kidney filtration, which shortens circulation time [4]. This study aimed to develop ⁶Li-doped CDs, encapsulated within core-shell nanoparticles (CSNPs) via a microfluidic nanofabrication technique, with the goal of producing CSNPs in the precise size range of 100-200 nm to enhance CD delivery by extending circulation time [5]. Following a hydrothermal reaction involving lithium chloride, urea, and citric acid, the resulting CDs were purified and analysed through UV-Vis spectroscopy, then dissolved in a BSA solution. Using a coflow system, this solution was introduced into a continuous ethanol flow, with a side stream of diluted glutaraldehyde, and then subjected to a dual (chemical and thermal) crosslinking process. The obtained CSNPs were characterized by SEM, TEM, DLS, and Zeta potential analysis. Our results showed that the developed microfluidics system enabled the precise nanofabrication of highly stable BSA-based nanocomposites with a controlled and narrowly distributed size profile.

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Workshop 2.

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2nd Workshop on ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES (19 November 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.

Topics:

Advanced materials

- Multifunctional Smart Materials
- 2D and Nanomaterials
- Polymers, Composites, Liquid crystals
- Photonic crystals and Metamaterials

Advanced technologies and applications

- Soft Robotics and Biomedical applications
- 3D Printing and Additive Manufacturing
- Optoelectronics and Energy applications
- Green technologies and sustainable manufacturing

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2nd Workshop on ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES (19 November 2024)

Plenary sessions							
Opening words 09:30 Chair: Indrani Coondoo							
09:35 - 10:15	Prof. Anil Kumar Department of Mechanical Engineering, Delhi Technological University, Delhi, India Advancement in Energy Storage Materials Integrated Solar Drying Systems Plenary lecture						
10:15 - 10:45	Prof. Majid Taghavi Department of Bioengineering, Imperial College London, London, UK Artificial muscles with extended functions for monolithic medical robots Plenary lecture						
10:45 - 11:30	 Prof. Satyaprakash Sahoo Laboratory for Low Dimensional Materials, Institute of Physics, Bhubaneswar, India Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai, India Emerging 2D quantum materials for brain-inspired neuromorphic computing applications Plenary lecture 						
Keynote sessions Chair: Ajeet Kumar							
11:30 – 12:00	Dr. Sugato Hajra Daegu Gyeongbuk Institute of Science and Technology, Daegu, South Korea Self-Powered Sensors using Triboelectrification Keynote talk						
12:00 – 12:30	Dr. Daniela V. Lopes CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Aveiro, Portugal Advancements in alkaline electrolysis for sustainable steelmaking technology and emerging hydrogen electrocatalysts Keynote talk						

Lunch Break						
14:00 – 14:15	Chair: Indrani Coondoo Tiago Rodrigues Physics Center of Minho and Porto Universities (CF-UM-UP), University of Minho, Campus de Gualtar, Braga, Portugal Laboratory of Physics for Materials and Emergent Technologies, LapMET, University of Minho, Braga, Portugal Strain-Driven Polar Topologies in SrTiO ₃ -δ Thin Films Oral presentation					
14:15 – 14:30	Sunny Choudhary Department of Physics, University of Puerto Rico at Río Piedras, San Juan, USA Encapsulation Engineering of Sulfur into Magnesium Oxide for High Energy Density Li–S Batteries Oral presentation					
14:30 – 14:45	Noelle C. Zanini Department of Materials and Ceramic Engineering, CICECO – Aveiro Institute of Materials, University of Aveiro, Aveiro, Portugal Dynamic Response of Lead-free Composite Flexible Generator for Sustainable Blue Energy Solutions Oral presentation					

2nd Workshop on ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES 19 November 2024, University of Aveiro, Portugal

Plenary lecture

Advancement in Energy Storage Materials Integrated Solar Drying Systems Anil Kumar

Head of Division-Clean Energy: Nodal Centre of Excellence in Energy Transition (NCEET)

Professor: Department of Mechanical Engineering

Delhi Technological University, Delhi-110 042 (India)

Integrating energy storage materials with solar drying systems has emerged as a promising solution to address the intermittent nature of solar energy and enhance the efficiency of drying processes. This expert talk explores recent advancements in energy storage technologies, specifically focusing on materials that can be seamlessly integrated into solar drying systems. Various energy storage solutions are examined for their potential to store excess solar energy generated during peak sunlight hours and release it during periods of low or no sunlight. The paper highlights the thermal properties of these materials, their capacity for efficient energy storage, and the ways they can optimize the performance of solar dryers by maintaining a consistent drying temperature. The challenges and limitations of each material, including cost, longevity, and scalability, are also discussed. Furthermore, the review assesses the environmental benefits of integrating energy storage into solar drying systems, particularly in agricultural and food processing industries, where energy-efficient drying methods can reduce post-harvest losses. It concludes with a look at future trends and research directions aimed at improving energy storage materials and their integration into solar drying technologies for sustainable, off-grid drying solutions.

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Plenary lecture

Artificial muscles with extended functions for monolithic medical robots Majid Taghavi

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The traditional robotic paradigm involves integrating discrete essential components for actuation, sensing, and energy, and designing effective control algorithms to achieve specific functions. This approach is not practical for soft robots, composed of compliant materials, due to two main limitations. First, the dissimilar properties of the underlying materials (such as rigid and soft materials, or electrodes and insulators) cause material, mechanical, and electrical mismatches, making its seamless integration too challenging. Second, due to the compliance and unlimited degrees of freedom in soft robotic components, their behavior is significantly affected when integrated with other components, necessitating an iterative design and optimization process to develop a new system and complex control architecture.

In this talk, I will present our approach to developing future monolithic soft robots for healthcare applications through the development of the next generation of artificial muscles with extended functionalities. I will discuss our strategy for investigating multifunctionality at the material, structural, and functional levels, incorporating features such as variable stiffness, graded stiffness, self-sensing, self-powering, adaptability, and shape-shifting in soft actuators. These features aim to establish novel core technologies for future wearable and implantable robotics.

2nd Workshop on ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES 19 November 2024, University of Aveiro, Portugal

Plenary lecture

Emerging 2D quantum materials for brain-inspired neuromorphic computing applications

Satyaprakash Sahoo^{1,2}

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In the era of big data and artificial intelligence the traditional Von-Neumann computing architecture is periodically confronted. Brain inspired Neuromorphic computing architecture integrated with in-memory computing capability could instigate unprecedented breakthroughs in AI technology. Although there has been progress in Neuromorphic computing, however, engineering the material aspect for its architecture remains a challenge. In this regard, the two-dimensional (2D) layered materials, consisting of atomically-thin layers, possess a plethora of exotic properties and have emerged as the leading contenders for the next generation of electronic devices. Specific attention has been given to the layered transition metal di-chalcogenides (TMDCs), has created numerous prospects for developing low-power electronics, cutting-edge memory device arrays and smart computing architectures with desirable miniaturization. In this talk I will discuss two approaches for achieving Neuromorphic computing with monolayer TMDCs mem-transistors; optoelectronic and thermal driven ionotronic approach. Twodimensional TMDC transistors demonstrating optoelectronic artificial synapse and reconfigurable logic operation are fabricated. The persistent photoconductivity of these devices are used to achieve the long- short term synaptic plasticity behaviour. Furthermore, Pavlov's classical conditioning is demonstrated by using the broadband sensitivity of the devices. More importantly, reconfigurable Boolean logic gate operations are demonstrated within the same device. We also demonstrate a novel mem-transistor device using monolayer TMDCs as channel that offers multi-bit high density storage states and can perform key synaptic operations above room temperature. This novel integration of memory, synaptic behaviour, and processing within a single monolayer TMDC device put forth a new horizon for the Non-Von-Neuman type in-memory computing architecture for advanced AI applications at room temperature and beyond.

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2nd Workshop on ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES 19 November 2024, University of Aveiro, Portugal

Keynote talk

Self-Powered Sensors using Triboelectrification Sugato Hajra^{*}, Hoe Joon Kim

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The development of self-powered devices has gained significant attention in recent years, particularly in the field of sensing applications. Triboelectrification, the process that occurs when two materials come into contact and transfer charge, serves as the foundation for creating devices with self-powered sensing capabilities. By leveraging electrostatic induction alongside triboelectrification, researchers have designed Triboelectric Nanogenerators (TENGs) for energy harvesting. Various aspects of triboelectric nanogenerator performance improvement strategies, hybrid energy harvesters will be discussed. Recent advancements have led to the development of solid-liquid TENGs. These improvements address the limitations of previous solid-solid TENGs , while also establishing new sensing mechanisms and principles critical to the field. The progress in developing TENGs suggests promising applications for future research, with potential use cases in both environmental and biological monitoring, offering a new frontier for many types of self-powered systems. This abstract summarizes the key advances and future directions in triboelectric-based sensing technology.

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2nd Workshop on ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES 19 November 2024, University of Aveiro, Portugal

Keynote talk

Advancements in alkaline electrolysis for sustainable steelmaking technology and emerging hydrogen electrocatalysts

Daniela V. Lopes^{1,*}, Aleksey D. Lisenkov¹, Sergii Sergiienko¹, Nuno F. Santos², Jorge P. Moura², António J.S. Fernandes², Florinda M. Costa², Andrei V. Kovalevsky¹

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The steel industry has a major impact on the global economy. However, iron is still traditionally produced via sequential carbothermal reductions in blast-furnace-basic-oxygen furnaces (BF-BOF), contributing 7 to 9% of global CO₂ emissions [1]. Alkaline electrowinning, an electrolysis-based technology, offers a promising CO₂-lean alternative to transform the industry. With lower operating temperatures (~100 °C) and energy consumption (~10 GJ/ton Fe) [2], this approach has minimal environmental impact due to the production of H₂ and O₂ as by-products from alkaline water splitting. Although alkaline electrolysis is an established technology for H₂ evolution, the electrolysis of iron oxides into Fe has been discredited due to the insulating behavior of Fe₂O₃, the main composition studied. Additionally, the hydrogen evolution reaction (HER) negatively impacts the Fe electrodeposition. This study provides an overview of the advancements in this technology, drawing from literature and case studies conducted by the authors.

Several concepts of ceramic cathodes and ceramic suspensions have shown promising results for both Fe₂O₃ and Fe₃O₄, as well as iron (hydro)oxides, achieving high Faradaic efficiencies (65-90%). The presence of non-conductive phases (e.g. Al-, Mg-, Ti-) as impurities was also tested and found to suppress electroreduction to Fe, to some extent. However, incorporating such impurities into iron-oxide-based matrices is a crucial approach to adapting this technology for a broader range of raw materials, such as industrial residues, with a relevant impact on the circular economy and industrial symbiosis.

Despite the negative impact of HER on Fe electrodeposition, there is potential to integrate it with Fe production, as the H₂ market is rapidly growing in Portugal. Emerging electrocatalysts for HER such as laser-induced graphene (LIG) and MXenes, a class of 2D materials, have also been explored showing promising results. Alkaline electrolysis for H₂ and Fe production can easily align with intermittent renewable energy sources, driving technological advancements in both steel and H₂ sectors in the upcoming years, with direct impact in society.

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2nd Workshop on ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES 19 November 2024, University of Aveiro, Portugal

Strain-Driven Polar Topologies in SrTiO₃-δ Thin Films

<u>**Tiago Rodrigues**</u>^{1,2*}, José P. B. Silva^{1,2}, Fábio Figueiras³, M. R. Soares⁴, R. Vilarinho^{2,3}, J. Agostinho Moreira^{2,3}, Ihsan Çaha⁵, Francis Leonard Deepak⁵, Bernardo Almeida^{1,2}

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We report the successful induction of ferroelectric behavior in 10-nm thick epitaxially strained $SrTiO_3-\delta$ (STO- δ) thin films, grown via ion-beam sputtering onto Nb-doped $SrTiO_3$ (Nb) (001) substrates. By controlling oxygen vacancies during growth, and post-deposition annealing at 750 °C, we demonstrate a transition from paraelectric to ferroelectric behavior, driven by precise defect engineering and strain.

To understand the structural and polar characteristics of these films, we employed a combination of high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM), Raman spectroscopy, and high-resolution X-ray diffraction (HRXRD). High-angle annular dark-field scanning transmission electron microscopy imaging reveals polar nanoregions with non-trivial topological structures induced by oxygen vacancies. Raman spectroscopy and high-resolution X-ray diffraction confirm a strained tetragonal phase with a c/a tetragonality ratio of 1.005. These findings suggest that strain plays a significant role in stabilizing the ferroelectric state in STO- δ films, which are typically paraelectric in bulk form.

Macroscopic ferroelectricity was confirmed via polarization-electric field hysteresis loops, yielding a remnant polarization of ~0.4 μ C/cm², a maximum polarization of ~1.5 μ C/cm², and a coercive field of ~0.3 MV/cm. Additionally, scanning probe microscopy identified localized ferroelectric domains, further verifying the nanoscale ferroelectric properties of the samples.

This work provides a new pathway to explore and control polar topologies in ultrathin films through defect and strain engineering, paving the way for future applications in non-volatile memory devices and low-power electronics. The ability to induce and manipulate ferroelectric properties in films thinner than 10 nm opens opportunities for miniaturized devices, where the stabilization of polar structures could lead to enhanced device functionality. [1]

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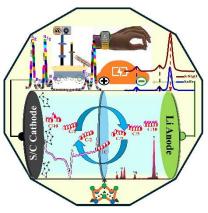
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Encapsulation Engineering of Sulfur into Magnesium Oxide for High Energy Density Li–S Batteries

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This research addresses the persistent problem of polysulfide dissolution in lithium–sulfur (Li–S) batteries by incorporating magnesium oxide (MgO) nanoparticles as an innovative additive. MgO was combined with sulfur using a scalable solid-state melt diffusion process, followed by planetary ball milling, to improve the electrochemical stability and performance of sulfur cathodes in high-energy-density Li–S batteries. The S-MgO composite was characterized through X-ray diffraction (XRD), Raman spectroscopy, and scanning electron microscopy (SEM). Electrochemical



assessments, such as cyclic voltammetry (CV), galvanostatic charge-discharge cycling, and electrochemical impedance spectroscopy (EIS), were performed to assess battery performance and stability.

XRD measurements confirmed that sulfur (S8) retains its orthorhombic crystalline structure (space group F_{ddd}) after MgO incorporation, with minimal peak shifts indicating slight lattice distortion, while the increased peak intensity suggests enhanced crystallinity due to MgO acting as a nucleation site. Additionally, Raman spectroscopy demonstrated sulfur's characteristic vibrational modes consistent with group theory (point group D_2h) and highlighted multiwalled carbon nanotube (MWCNT's) D, G, and 2D bands, with a low ID/IG ratio (0.47), which indicated low defects and high crystallinity in the prepared cathode. The S-MgO composite cathode exhibited superior electrochemical behavior, with an initial discharge capacity (950 mA h g⁻¹ at 0.1C), significantly improved than pristine sulfur's. The presence of MgO effectively mitigated the polysulfide shuttle effect by trapping polysulfides, leading to enhanced stability over 400 cycles and a consistent coulombic efficiency of over 99.5%. After 400 cycles, EDS and SEM analyses confirmed the structural integrity of the electrode, with only minor fractures and slight sulfur content loss.

Overall, MgO effectively mitigated the polysulfide shuttle effect by trapping polysulfides, resulting in enhanced cycle stability and higher sulfur utilization. These findings highlight MgO's potential as an additive for improving long-term stability in Li–S batteries, positioning the composite as a promising candidate for future energy storage applications, including space exploration, where durability and energy density are critical.

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2nd Workshop on ADVANCED MATERIALS: APPLICATIONS AND TECHNOLOGIES 19 November 2024, University of Aveiro, Portugal

Dynamic Response of Lead-free Composite Flexible Generator for Sustainable Blue Energy Solutions

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In the quest to design flexible energy harvesters capable of operating in unpredictable, force-variable environments, understanding the combined effects of frequency and applied force is essential to optimizing their energy output and efficiency [1]. This work aims to fabricate a lead-free composite flexible generator to harvest renewable energy to power small devices in future blue energy applications. We fabricated these composites by mixing polydimethylsiloxane (PDMS) with 30 wt.% potassium-sodium niobate (KNN) and 2 wt.% graphite (G) with further curing and simultaneous poling of the mixture at 80 °C under 5 kV for 30 min followed by assembling copper tape on the composite (PDMS/KNN/G) surfaces and polyethylene packaging to have a generator. The composite was characterized using thermogravimetric analysis, tensile test, contact angle (CA), water absorption, scanning electron microscopy (SEM), and energy-dispersive Xray spectroscopy (EDS) techniques. The generator electrical output was stimulated by a shaker in a frequency range of 5-100 Hz and applied force range of 1-5 N and measured in the top face mode with a load resistance of 5 M Ω . The PDMS/KNN/G demonstrated thermal resistance up to 250 °C, flexibility with a low Young Modulus of 1.2 MPa, a low wettability with a contact angle of 106 ° and low water absorption after one week of immersion in distilled water (0.5%). The fillers were prominent at the top face of the composite film according to the SEM/EDS micrographs. The influence of force applied at different frequencies was analyzed by the root mean square voltage (V_{rms}) trend lines. An increase in the force applied to the generator top face intensified the V_{rms} output seen by the trend line slope [2]. The same behavior was observed for the frequency [3], with the highest V_{rms} of 147 mV at 100 Hz and 5 N. The observed increase in V_{rms} with heightened force and frequency demonstrates the generator's potential to provide reliable power for small-scale electronic devices, highlighting its viability as a renewable energy source for applications in blue energy solutions.

Acknowledgments

This work was developed within the ECIU-FCT scholarship (PRT/BD/154320/2023), with the Aalborg University and within the scope of the project CICECO-Aveiro Institute of Materials, UIDB/50011/2020, UIDP/50011/2020 & LA/P/0006/2020, financed by national funds through the FCT/MCTES (PIDDAC).

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Workshop 3









Funded by the European Union NextGenerationEU

Workshop on Challenges and Strategies in Degradation of Organic Contaminants Research

SMALL MOLECULES, BIG PROBLEMS

The production and constant use of various products present urgent and significant environmental challenges, causing considerable harm to living organisms. Despite efforts in water treatment, many organic contaminants have accumulated in the environment. These contaminants break down into degradation by-products under environmental conditions. Their small size, high stability, and slow decomposition make them a serious environmental concern.

The workshop aims to highlight the challenges and pitfalls in organic contamination research and explore effective methods for their removal from the environment. It will serve as a roundtable for presenting new findings and discussing them with the audience, providing a valuable opportunity to contribute to and enhance current research

The organizing committee warmly invites you to participate in our upcoming Workshop on Challenges and Strategies in the Research of Organic Contaminant Degradation, which will focus on innovative research shaping the future of materials science.



19.11.2024.



Online Mode



Students, researchers, and anyone interested in the field of materials engineering



No registration fees. Participation is free.



Organizing committee:

Prof. Dr. Aleš Omerzu, University of Rijeka, Croatia
M.Sc. Damjan Vengust, Jožef Stefan Institute, Slovenia
M.Sc. Daria Jardas Babić, University of Rijeka, Croatia
Prof. Dr. Iva Šarić Janković, University of Rijeka, Croatia
Prof. Dr. Ivna Kavre Piltaver, University of Rijeka, Croatia
Dr. Martina Kocijan, University of Rijeka, Croatia
Dr. Matejka Podlogar, Jožef Stefan Institute, Slovenia
Prof. Dr. Robert Peter, University of Rijeka, Croatia
M.Sc. Tina Radošević, Jožef Stefan Institute, Slovenia
Prof. Dr. Ivana Jelovica Badovinac, University of Rijeka, Croatia
Dr. Marija Egerić, Vinča Institute of Nuclear Sciences, Serbia



Workshop Contact:

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Workshop on Challenges and Strategies in Degradation of Organic Contaminants Research

Workshop program

15:00 - 15:10	WELCOME ADDRESS Prof. Ivna Kavre Piltaver Dr. Matejka Podlogar, Dr. Martina Kocijan			
CHAIR: MSc. Tina Radošević				
15:10 - 15:30	MSc Daria Jardas Babić Faculty of Physics and Centre for Micro- and Nanosciences and Technologies, University of Rijeka, Croatia <i>Title:</i> Atomic Layer Deposition of Semiconductor Thin Films for Photocatalytic Applications			
15:30 - 15:50	Prof. Aleš Omerzu Faculty of Physics and Centre for Micro- and Nanosciences and Technologies, University of Rijeka, Croatia <i>Title:</i> Thin ZnO films prepared by plasma-enhanced atomic layer deposition (PEALD) for future photocatalytic applications			
15:50 - 16:00	Coffee break			
CHAIR: Dr. Martina Kocijan				
16:00 - 16:20	Dr. Matejka Podlogar Department for Nanostructured Materials, Jožef Stefan Institute, Ljubljana, Slovenia <i>Title:</i> Modifying the defect population in ZnO nanorods through solvothermal synthesis for enhanced photocatalytic performance			
16:20 - 16:40	Dr. Marija Egerić Vinča Institute of Nuclear Sciences, Beograd, Serbia <i>Title:</i> Degradation of organic pollutants by gamma irradiation: progress in wastewater treatment			
16:40 - 17:00	Final discussion and comments			

Atomic Layer Deposition of Semiconductor Thin Films for Photocatalytic Applications

Daria Jardas Babić^{*1}, Ivana Jelovica Badovinac¹, Ivna Kavre Piltaver¹, Iva Šarić Janković¹, Robert Peter¹, Aleš Omerzu¹

¹University of Rijeka, Faculty of Physics & Centre for Micro- and Nanosciences and Technologies, Rijeka, Croatia

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In this talk I will present our research equipment for the synthesis and analysis of photocatalytic materials. For the synthesis we use atomic layer deposition (ALD), a developed technique for producing thin, uniform films layer by layer. In addition to the general principles of ALD, I will also explain the capabilities of our ALD system. To characterize the synthesized material, we determine its structural and chemical composition using advanced experimental techniques. X-ray photoelectron spectroscopy (XPS) allows a detailed analysis of the chemical composition of the surface by detecting elements and identifying their chemical states, which is essential in areas such as photocatalysis. Scanning electron microscopy (SEM) is used to visualize material morphology and elemental analysis (EDS) can be used to determine the chemical composition of a sample. For even more precise in-depth analysis, secondary ion mass spectrometry (SIMS) offers highly sensitive element detection that can even detect trace amounts through layers. SIMS is particularly valuable for studying multilayer structures and changes in composition with depth, which is crucial in thin films. Together, these instruments provide a comprehensive understanding of material properties, which is essential for improving the photocatalytic performance of the material under study.

Acknowledgments

We acknowledge the support of core funding from NPOO.C3.2.R2-I1.06.0083, provided by the European Union's NextGenerationEU initiative and project grants 23-190 and 23-4 from the University of Rijeka.

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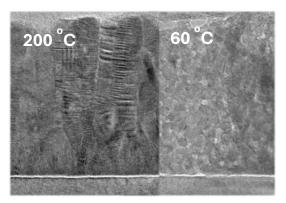
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Thin ZnO films prepared by plasma-enhanced atomic layer deposition (PEALD) for future photocatalytic applications

<u>Aleš Omerzu</u>¹, Daria Jardas Babić¹, Robert Peter¹, Krešimir Salamon², Tina Radošević³, Damjan Vengust³, Matejka Podlogar³

¹ Faculty of Physics and Centre for Micro- and Nanosciences and Technologies, University of Rijeka, Rijeka 51 000, Croatia
² Ruđer Bošković Institute, Bijenička cesta 54, Zagreb 10 000, Croatia
³ Jožef Stefan Institute, Jamova 39, Ljubljana 1000, Slovenia
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Atomic layer deposition (ALD) is an advanced deposition technique that allows us to synthesize high-guality thin ZnO films. By varying the parameters for thin film synthesis, different structural and physical properties of the films can be obtained [1-4]. The most important synthesis parameter is the deposition temperature. In thermal ALD, the temperature range for the deposition of highquality films is between 120 °C and 180 °C. An upgrade of conventional ALD is plasma-



enhanced atomic layer deposition (PEALD), which enables deposition at lower temperatures without impairing the film quality and growth rate. The photocatalytic activity of the films deposited by the PEALD method shows a maximum value for films deposited at temperatures below 100 °C, and their efficiency is higher than that of the best thermal ALD films. In the present study, we compared the crystal structure, optical properties and photocatalytic activity of thin films deposited at 60°C, 80°C, 100°C and 200°C using the PEALD method. The TEM images show that the films synthesized at lower temperatures have smaller, roundish grains, while the films synthesized at higher temperatures consist of larger, elongated crystals that are perpendicular to the substrate. The smaller grain structure has a much higher concentration of localized surface states, resulting in better photocatalytic activity.

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Modifying the defect population in ZnO nanorods through solvothermal synthesis for enhanced photocatalytic performance

Matejka Podlogar^{1*}, Patrick Seleš¹, Damjan Vengust¹, Tina Radošević¹,

Martina Kocijan², Lara Einfalt¹, Mario Kurtjak¹, Vasyl Shvalya¹, Tilen Knaflič¹,

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Zinc oxide's high abundance and low toxicity make it highly attractive for photocatalytic applications in water remediation. Its performance can be enhanced by inducing native defects in ZnO nanocrystals, but conventional high-temperature post-processing often results in grain agglomeration and crystal growth. This study demonstrates that defect populations can be tuned during the recrystallization process by optimizing conditions. ZnO nanorods derived from nanodots were tested for degrading caffeine as a model pollutant. The synthesized powders were characterized using XRD, SEM, TEM, and BET techniques. Defects were analyzed using Raman, photoluminescence, and EPR spectroscopy, while surface chemistry was studied via XPS. Surprisingly, photocatalytic efficiency was found to be governed by bulk defect populations rather than surface chemistry.

Acknowledgments: We acknowledge the support of ARIS through projects L2-1830, BI-HR/20-21-003, and program P2-0084.

Degradation of Organic Pollutants by Gamma Irradiation: Progress in Wastewater Treatment

<u>Marija Egerić</u>^{1,2*}, Radojka Vujasin¹, Srboljub Stanković¹, Sanja Krstić¹, Aleksandar Devečerski¹, Ljiljana Matović^{1,2,3}

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Organic pollutants may originate from different sources and, even in small concentrations, have a negative impact on the environment, due to the rapid development of various industries. Traditional wastewater treatment methods are often insufficient for the complete degradation of these compounds, creating a need for alternative approaches. This study reviews recent achievements in the gamma irradiation application for wastewater treatment, focusing on diverse organic pollutants, such as dyes, pesticides and antibiotics. The interaction between water molecules and gamma rays results in water degradation and generation of the oxidizing active species, hydroxyl and perhydroxyl radicals. Documented by-products, typically less toxic than the original pollutants, can often be further degraded with higher irradiation doses. To avoid the application of high irradiation doses and to improve the degradation process, coupling with different techniques was investigated, including oxidizing agents [1], solid matrices (solid-liquid systems) [2], biological treatment [3] or gamma irradiation-modified materials [4]. The application of gamma irradiation in modular or mobile treatment units could offer a practical solution for large-scale wastewater treatment, contributing to sustainable water resource management and reduced environmental impact.

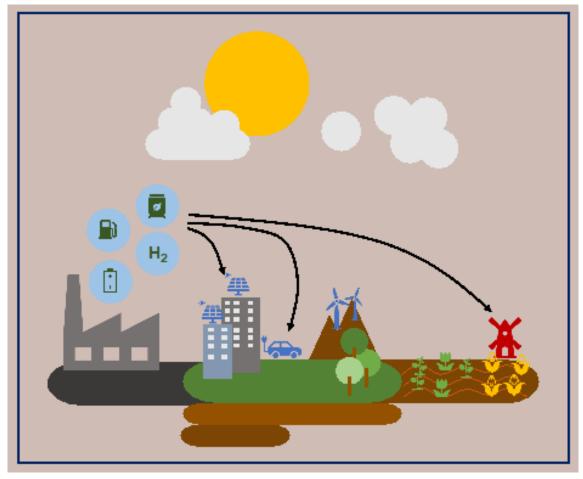
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Workshop 4



3rd International Workshop on "Modern Trends in Energy Research" 19 November 2024, Aveiro, Portugal



Topics:

Green Hydrogen: Production, Storage & Transport

Fuel Cells/Electrolysers

Electrochemical Synthesis of Green Fuels and Chemicals

Batteries & Supercapacitors

Nanocatalysis & Electrocatalysts







Convener: Dr. D. Pukazhselvan (UA, Portugal)

Co-convener: Dr. Francisco Loureiro (UA, Portugal)

Host Institution: Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal.

Local Organizing committee:

Dr. D. Pukazhselvan (UA, Portugal)Dr. Igor Bdikin (UA, Portugal)Dr. Duncan Paul Fagg (UA, Portugal)Dr. Francisco Loureiro (UA, Portugal)

*No registration fee

*This event is only in online mode

Workshop Contact: dpukazh@ua.pt

Deadline for abstract submission: 10th November 2024

Abstract format: Any format in word / pdf (1 page)

Length of each lecture: 15 to 30 minutes







3rd International Workshop on Modern Trends in Energy Research 19 November 2024, University of Aveiro, Portugal

Session 1: 9.00 to 10.15 h Session Chair: Duncan Paul Fagg / Francisco Loureiro

9.00 to 9.20: **D. Pukazhselvan (welcome address and keynote lecture)** TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal *Title: Introduction to energy crisis and probable solutions*

W4-PL1

9.20 to 9.45: Bruno Melo (plenary lecture) Department of Physics, University of Aveiro, Portugal *Title: Solid acid composites as electrolytes for intermediate temperature fuel cells*

W4-I1

9.45 to 10.00: Olena Okhay (Invited talk)

TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal *Title: Supercapacitor electrodes based on reduced graphene oxide by various*

methods

W4-I2

10.00 to 10.15: **Ihsan Çaha (Invited talk)**

International Iberian Nanotechnology Laboratory, Braga, Portugal Title: Multi-Scale Characterization of NMC111 Cathodes for Li-ion Batteries: From Atomic Structure to Electrode Architecture with 4D STEM and FIB-SEM

Session 2: 10.30 to 11.30h Session Chair: Vanessa Graca

W4-I3 10.30 to 10.50: **Sathishkumar Duraisami (Invited talk)** TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal *Title: Optimisation of electron beam welding parameters for copper pipe joints in heat pump systems*

W4-I4

10.50 to 11.15:Fausthon Fred da Silva (Invited talk)Chemistry Department, Federal University of Paraíba, BrazilTitle: Boosting the Electrocatalytic Activity of Metal-Organic Frameworks DerivedMetal-Oxide Nanoparticles in Oxygen Evolution Reaction

W4-I5

11.15 to 11.30:Alfredo S. B. Luemba (Invited talk)Department of Mechanical Engineering, University of Aveiro, PortugalTitle: Development of novel proton-conducting materials for ceramic fuelcells/electrolyzers





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3rd International Workshop on "Modern Trends in Energy Research" 19 November 2024, University of Aveiro, Portugal

Session 3: 11.30 to 12.30h

Session Chair: Laura Holz

	W5-I6			
11.30 to 11.50: Sivabalan Maniam Sivasankar (Invited talk)				
Department of Physics, i3N, University of Aveiro, Portugal				
Title: Interface and surface engineering of CIGS films to improve cell				
performance				
	W5-I7			
11.50 to 12.05: Lara F. Almeida Paiva (Invited talk)				
TEMA - Centre for Mechanical Technology and Automation, Department of				
Mechanical Engineering, University of Aveiro, Portugal				
Title: A robust hydrothermal synthesis method of $NH_4Zr_2(PO_4)_3$, a precursor f	or			
$HZr_2(PO_4)_3$ proton conductor				
	W5-18			
12.05 to 12.20, Vivok Chukle (Invited talk)	VVJ-10			
12.05 to 12.30: Vivek Shukla (Invited talk)				
Centre for Hydrogen Energy Materials, Korea Institute of Science and Technology,				
Seoul, 02792, Republic of Korea				
Seoul, 02792, Republic of Korea Title: Hydrogen sorption characteristics of Ti-Al-O ternary system				







FC'

3rd International Workshop on "Modern Trends in Energy Research" 19 November 2024, University of Aveiro, Portugal

Keynote lecture

Introduction to energy crisis and probable solutions D. Pukazhselvan^{1,2,*}

¹TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal
²LASI - Intelligent Systems Associate Laboratory, 4800-058 Guimarães, Portugal
³LAQV-REQUIMTE, Department of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, Rua do Campo Alegre, s/n, 4169-007, Porto, Portugal E-mail: dpukazh@ua.pt

The depletion of fossil fuels and the rising levels of CO2 in the atmosphere are two of the most pressing challenges on the planet today [1]. In 2015, the concentration of CO2 in the atmosphere surpassed the dangerous threshold of 400 ppm. As of October 2024, the CO2 concentration has reached 422.4 ppm, marking a significant increase compared to the figure recorded one year earlier, when it was 418.8 ppm in October 2023. Recent years have seen considerable progress in the European Union regarding electricity production from renewable energy sources. However, these advancements will only make a real impact if renewable energy can be effectively harnessed for vehicles, which necessitates a specific amount of stored energy on board. To address the energy storage needs for vehicles, researchers around the world have proposed four alternative options: (i) bio-hydrocarbons coupled with a CO2 sequestration cycle, (ii) ammonia as a direct fuel, (iii) hydrogen as a fuel, and (iv) batteries for electric energy storage. Among these options, hydrogen and batteries are regarded as the most promising. However, both face significant challenges, for example, (i) the capacity of modern lithium-ion batteries needs substantial enhancement beyond current optimization levels, and (ii) hydrogen vehicles require improved hydrogen storage materials capable of releasing hydrogen reversibly under affordable operating conditions. The energy research team at the University of Aveiro (TEMA) has optimized various lithium and hydrogen storage materials [2]. Our findings indicate that lithium batteries with modified carbon anodes and metal hydride systems using modified MgH2 could make long-range lithium and hydrogen-powered vehicles a practical reality.

Acknowledgement: This article was supported by the projects UIDB/00481/2020 and UIDP/00481/2020 - Fundação para a Ciência e a Tecnologia, DOI 10.54499/UIDB/00481/2020 (https://doi.org/10.54499/UIDB/00481/2020) and DOI 10.54499/UIDP/00481/2020 (https://doi.org/10.54499/UIDP/00481/2020). D. P acknowledges FCT, Portugal for the financial support reference CEECIND/04158/2017 with (https://doi.org/10.54499/CEECIND/04158/2017/CP1459/CT0029). The authors are also grateful for the financial support granted by the Recovery and Resilience Plan (PRR) and by the Next Generation EU European Funds to Universidade de Aveiro, through the Agenda for Business Innovation "NGS -Next Generation Storage" (Project no 02/C05-i01.01/2022 with the application C644936001-00000045).

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3rd International Workshop on "Modern Trends in Energy Research" 19 November 2024, University of Aveiro, Portugal

Plenary lecture

W4-PL1. Solid acid composites as electrolytes for intermediate temperature fuel cells

<u>Bruno Melo^{1,*},</u> Francisco Loureiro^{2,3}, Sergey Mikhalev^{2,3}, Duncan Fagg^{2,3}, Luís C. Costa¹, Manuel Graça¹

 ¹ i3N, Department of Physics, University of Aveiro, 3810-193 Aveiro, Portugal
 ² TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal
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The extensive reliance on fossil fuels such as coal, oil, and natural gas in recent decades has led to significant air pollution and the depletion of vital oil reserves. Beyond posing serious health risks, the mining and combustion of these fuels produce carbon dioxide emissions, a key contributor to climate change and other environmental issues. Fuel cells have emerged as one of the most promising hydrogen-based technologies for sustainable energy conversion. However, there remains a demand for intermediate temperature fuel cells that can operate effectively within the 200-500 °C range, as these could bridge the gap between low and high temperature fuel cells and address current challenges, such as reducing the need for non-metal catalysts, lowering costs, and enhancing longevity. In this study, we prepared a series of $CsH_2PO_4-CsH_5(PO_4)_2$ composite systems aimed at enhancing the electrical conductivity of the electrolyte at sub-transition temperatures. Thermal stability was evaluated using Thermogravimetric and Differential Thermal Analysis (TGA/DTA) on a Hitachi STA 7300, with measurements conducted under a nitrogen (200 mL/min, N50, 99.999%) atmosphere at a heating rate of 10 °C/min. Electrochemical Impedance Spectroscopy (EIS) was performed using an Autolab PGSTAT302N potentiostat/galvanostat, covering a frequency range from 0.1 Hz to 1 MHz with a 200 mV signal amplitude. Sample morphology was examined via Scanning Electron Microscopy (SEM) on a Hitachi Tabletop microscope TM4000 Plus, and X-ray diffraction patterns were obtained using a Shimadzu 7000 diffractometer (CuKa radiation, 40 kV and 40 mA) over a 20 range of 10° to 80°, scanned at 2° per minute. This comprehensive analysis provides insights into the structural and electrochemical properties of CsH₂PO₄ composites, contributing to the development of efficient electrolytes for intermediate-temperature fuel cells.

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3rd International Workshop on "Modern Trends in Energy Research" 19 November 2024, University of Aveiro, Portugal

Invited talk

W4-I1. Supercapacitor electrodes based on reduced graphene oxide by various methods

Olena Okhay ^{1,2*}, Alexander Tkach³

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²LASI—Intelligent Systems Associate Laboratory, Guimaraes, Portugal

³CICECO-Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Portugal

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Similar to energy harvesting, energy storage is one of the most important topics of scientific research today due to the widespread use of both small batteries in watches, phones, computers, and large supercapacitors/batteries in cars, etc. [1]. Similar to monolayer graphene with ideal properties in various fields, the reduced graphene oxide (rGO) is a promising material for improving the structural and electrochemical properties of capacitive electrodes of energy storage devices, namely supercapacitors and batteries [2]. Meanwhile, aerogel-like rGO, which is lightweight and can have a large surface area, is a more promising material for energy storage compared to dense rGO membranes obtained by vacuum filtration. At the same time, the process of preparing rGO, as well as composite materials based on rGO, plays a significant role in the final characteristics of the material and the device. Dense free-standing rGO electrodes obtained by vacuum filtration are compared with composite electrodes made from rGO powder or aerogel on a different substrate.

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3rd International Workshop on "Modern Trends in Energy Research" 19 November 2024, University of Aveiro, Portugal

Invited talk

W4-I2. Multi-Scale Characterization of NMC111 Cathodes for Li-ion Batteries: From Atomic Structure to Electrode Architecture with 4D STEM and FIB-SEM

Ihsan Çaha and Francis Leonard Deepak

International Iberian Nanotechnology Laboratory-INL Braga, Portugal

The advancement of Li-ion batteries (LIBs) depends on a comprehensive understanding of cathode materials at multiple scales, from atomic structure to electrode architecture. This study presents a multi-scale characterization of NMC111 (LiNi_{0.33}Mn_{0.33}Co_{0.33}O₂) cathode materials, integrating atomic and microscale analyses to provide detailed structural, compositional, and morphological insights essential for optimizing battery performance. Employing 4D Scanning Transmission Electron Microscopy (4D STEM) and Focused Ion Beam-Scanning Electron Microscopy (FIB-SEM), we characterize both individual particle properties and the full electrode assembly.

At the atomic scale, 4D STEM facilitated an in-depth analysis of crystallographic orientation, phase distribution, and strain mapping within single NMC111 particles, offering unprecedented clarity on atomic arrangement and strain behavior. This approach, including differential phase contrast (DPC) imaging for visualizing light elements like lithium, enabled a detailed understanding of intrinsic and extrinsic factors impacting electrochemical performance. High-resolution strain mapping further revealed lattice distortions and their correlation with phase transitions, critical for identifying degradation mechanisms in NMC materials.

In parallel, FIB-SEM was used to characterize a realistic electrode structure comprising NMC111 particles, carbon black, and polyvinylidene fluoride (PVDF) coating on an aluminum current collector. Employing the slice-and-view method, FIB-SEM facilitated a microscale analysis of particle distribution, porosity, and three-dimensional structural reconstruction. This provided key insights into electrode homogeneity and particle connectivity, crucial parameters for efficient ionic and electronic transport.

This multi-scale approach bridges the gap between atomic-level phenomena and large-scale electrode design, offering a robust understanding of the microstructural characteristics that govern LIB cathode performance. By combining 4D STEM's atomic-scale resolution with FIB-SEM's capability for three-dimensional architectural analysis, this work establishes a foundational framework for developing NMC-based cathodes with enhanced structural stability and electrochemical efficiency.





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3rd International Workshop on "Modern Trends in Energy Research" 19 November 2024, University of Aveiro, Portugal

Invited talk

W4-I3. Optimisation of electron beam welding parameters for copper pipe joints in heat pump systems

 Sathishkumar Duraisamy¹, *, João Dias¹, Antonio Bastos¹, Ana Horovistiz¹
 ¹Center for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal
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The global demand for heat pumps has significantly increased owing to their energy efficiency and environmental benefits. However, conventional manufacturing methods for heat pumps encounter challenges such as low production efficiency, high energy consumption, and adverse environmental impacts. This advanced welding method can significantly improve the production efficiency and quality of heat pump components, particularly in joining complex geometries and dissimilar materials.[1] The investigation focused on refining Electron Beam Welding (EBW) techniques for joining copper pipes in heat pump systems. Two experimental groups were evaluated: Group 1 employed reduced beam intensity and welding velocity, whereas Group 2 utilised elevated levels of these parameters. The findings revealed that Group 1 achieved superior thermal dissipation and comprehensive welds in contrast to Group 2, which displayed inadequate heat distribution and a multitude of flaws. However, both groups displayed satisfactory microstructures in the impact zone, and the key findings indicated that optimising the beam current and welding speed is crucial for achieving high-quality welds. Reducing both parameters led to significant improvements in weld quality, better heat distribution, and fewer defects. This study concludes that precise control of EBW parameters can result in more reliable and efficient heat pump manufacturing, providing valuable insights into the microstructural characteristics and mechanical properties of EBW joints and offering important reference points for adopting this technology in the heat pump industry. The implementation of EBW is expected to enhance the overall manufacturing processes and product quality in the heat-pump sector, potentially revolutionising the industry's approach to production.

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3rd International Workshop on "Modern Trends in Energy Research" 19 November 2024, University of Aveiro, Portugal

Invited talk

W4-I4. Boosting the Electrocatalytic Activity of Metal-Organic Frameworks Derived Metal-Oxide Nanoparticles in Oxygen Evolution Reaction

Fausthon Fred da Silva

Department of Chemistry, Federal University of Paraíba, Brazil

The imminent threat of climate change is leading to an acceleration of the change in the global energy matrix. Among the alternatives of clean and renewable sources, hydrogen gas (H₂) has stood out, however the synthesis of this vector is still a challenge. This gas can be obtained from the electrolysis of water which consists of two half-reactions, Hydrogen Evolution Reaction (HER) and Oxygen Evolution Reaction (OER). However, this process, especially OER, requires a high overpotential to occur, and it is necessary to use catalysts for this reaction to be viable. On the other hand, Metal-Organic Frameworks (MOFs) are porous crystalline materials applied in catalytic processes. Nanomaterials derived from MOFs have stood out in the literature, with high performance in OER. Within this context, this lecture will address some synthetic strategies for boosting the catalytic performance of metal-oxide nanoparticles applied as electrocatalysts for OER





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3rd International Workshop on "Modern Trends in Energy Research" 19 November 2024, University of Aveiro, Portugal

Invited talk

W4-I5. Development of novel proton-conducting materials for ceramic fuel cells/electrolyzers

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Proton Ceramic Fuel Cells (PCFCs) and Proton Ceramic Electrolysis Cells (PCECs) are advanced electrochemical devices capable of converting chemical energy directly into electricity or viceversa. These devices are promising for clean and efficient energy generation due to their high efficiency, fuel flexibility, and low environmental impact. They utilize solid-state proton-conducting materials, typically composed of perovskite proton conductors. Recently, stannate-based perovskites have shown great promise due to their high proton conductivity (10⁻² S cm⁻¹ at 600°C) in humidified conditions ($p_{H20} \sim 10^{-2}$ atm) [1]. Hence, they are promising choices as electrode components for PCFCs/PCECs. In this context, the current study explores a novel composite electrode composed of a barium stannate proton conductor and a metallic Ni component. Specifically, stannate-based proton-conducting materials BaSn_{0.80}Y_{0.20}O_{3-d} (BSYO3) and Ba₂SnO₄ (BSO4) were synthesized via a mechanochemical activation route. X-ray diffraction (XRD) confirmed the formation of pure phases for both compounds. Symmetrical cells with a Ni-BSO4||BSYO||Ni-BSO4 configuration were fabricated (40 vol%Ni), following a previously established procedure [2]. Electrochemical Impedance Spectroscopy (EIS) was conducted on these symmetrical assemblies to evaluate the electrochemical properties of the Ni-BSO4 electrode. Preliminary analysis of data collected under humidified hydrogen fuel ($p_{H2O} \sim 10^{-2}$ atm) identified three primary processes governing the electrode mechanism: (i) a high-frequency process associated with proton transfer across the electrode/electrolyte interface, (ii) an intermediate-frequency process linked to charge-transfer reactions at the triple phase boundaries, and (iii) a low-frequency process related to gas-phase conversion and diffusion. To our knowledge, this study introduces a new category of electrodes for prospective PCFC/PCEC applications.

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3rd International Workshop on "Modern Trends in Energy Research" 19 November 2024, University of Aveiro, Portugal

Invited talk

W4-I6. Interface and surface engineering of CIGS films to improve cell performance

Sivabalan Maniam Sivasankar¹, Carlos de Oliverira Amorim¹, Rui Ramos Ferreira e Silva², António F da Cunha¹

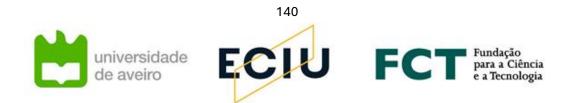
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This study explores the deposition and optimization of Copper Indium Gallium Selenide (CIGS) thin-film absorber precursors to advance second-generation photovoltaic technologies. CIGS, characterized by its tunable band gap $(1.0-2.4 \text{ eV})^1$, is a promising material for solar applications due to its efficient light absorption, stability, and potential for cost-effective production. The objective of this research was to establish a high-quality deposition process and evaluate the influence of various fabrication parameters on absorber quality and device performance.

The deposition procedure incorporated a custom-engineered sputtering system for the deposition of CIGS precursor layers, followed by one of two distinct annealing methodologies: in-situ chamber annealing and rapid thermal processing (RTP). The influence of each technique on the absorber's morphology, crystallinity, and compositional attributes was systematically evaluated. After deposition, comprehensive characterization was conducted employing Scanning Electron Microscopy coupled with Energy Dispersive X-ray Spectroscopy (SEM-EDX) for morphological and compositional assessments, X-ray Diffraction (XRD) to appraise crystallinity, and Glow Discharge Optical Emission Spectroscopy (GDOES) for depth-resolved elemental analysis, which facilitates the calculation of the absorber's band gap profile².

The study investigated conventional bi-layer stacking approaches, specifically Mo/CuGa/In and Mo/In/CuGa configurations, to evaluate their effectiveness in producing optimal CIGS layers. Results showed that placing CuGa in direct contact with the molybdenum back contact improved layer compactness but reduced overall cell performance. Conversely, the Mo/In/CuGa configuration, while exhibiting higher cell efficiency, suffered from poor adhesion due to void formation at the molybdenum interface, causing surface irregularities. These findings reveal a trade-off between adhesion quality and device efficiency, suggesting that precise control over precursor stacking is crucial for optimizing CIGS absorber properties.

The annealing conditions were discovered to have a profound effect on the structural integrity of the absorber. Although Rapid Thermal Processing (RTP) enhanced both compactness and morphological uniformity, it also presented a potential threat of substrate deformation and damage to the absorber layer. This underscores the necessity to establish a balance between improved material properties and maintaining structural robustness. In order to further enhance performance, an investigation into alkali metal doping through post-deposition treatment (PDT) was conducted utilizing sodium fluoride (NaF). The doping process resulted in an efficiency increase of approximately 1–2%. Notably, more substantial performance enhancements were observed when the NaF precursor was deposited on top of the molybdenum back contact before the deposition of CIGS. This approach offered the additional advantage of minimizing the number of necessary supplementary processing steps. This outcome underscores the significance of the doping sequence in optimizing efficiency gains.



GDOES analysis demonstrated that there is an accumulation of gallium at the rear of the absorber, which results in the formation of a graded band gap with a larger bandgap toward the rear of the absorber. This graded band gap profile is beneficial for the collection of charge carriers and diminishes recombination losses.

In conclusion, this study outlines a refined methodology for developing high-performance CIGS absorbers, emphasizing the roles of precursor stacking, annealing processes, and alkali doping. These findings contribute to advancing CIGS technology for broader application in sustainable energy, marking progress in optimizing thin-film solar cell efficiency and stability.

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3rd International Workshop on "Modern Trends in Energy Research" 19 November 2024, University of Aveiro, Portugal

Invited talk

W4-I7. A robust hydrothermal synthesis method of NH₄Zr₂(PO₄)₃, a precursor for HZr₂(PO₄)₃ proton conductor

Lara F. Almeida Paiva^{1*}, E. Durana², Laura I. V. Holz^{2,3}, Manuel P. F. Graça¹, Duncan P. Fagg^{2,3}

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Hydrogen zirconium phosphate (HZP), with the chemical formula HZr₂(PO₄)₃, exhibits promising properties such as anhydrous protonic conductivity, stability of intrinsic protons up to 650 °C, and high chemical resilience in both aqueous and acidic environments [1,2]. These characteristics make HZP a potential candidate for electrolyte applications, including gas separation, fuel cells, and electrolysers. However, research on HZP remains limited, primarily due to challenges in synthesizing the material in a pure phase.

To address this challenge, this study explores a new hydrothermal synthesis method designed to produce phase-pure ammonium precursor $NH_4Zr_2(PO_4)_3$, aiming to streamline the synthesis of HZP. This approach highlights the importance of precisely controlling reaction conditions to obtain pure $NH_4Zr_2(PO_4)_3$ in both its cubic and hexagonal polymorphs. For instance, a hydrothermal reaction at 150 °C with 2.1 mL of aqueous ammonia yields the cubic phase after 10 hours, whereas a temperature of 200 °C with 2.3 to 2.4 mL of aqueous ammonia promotes the formation of the hexagonal phase.

The study further investigates optimal conditions for converting hexagonal $NH_4Zr_2(PO_4)_3$ to hexagonal $HZr_2(PO_4)_3$ through thermal treatment at 600 °C for 5 hours, employing X-ray diffraction and infrared spectroscopy to assess phase purity and structure. This research aims to establish a robust synthesis pathway, enabling broader investigation and application of HZP.

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3rd International Workshop on "Modern Trends in Energy Research" 19 November 2024, University of Aveiro, Portugal

Invited talk

W4-I8. Hydrogen sorption characteristics of Ti-Al-O ternary system <u>Vivek Shukla</u>, Young-Su Lee

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To realize the functional hydrogen economy that includes production, storage, and application, hydrogen storage is crucial. The Ti-Al system has been considered a potential hydrogen storage material because it consists of one hydride-forming element, Ti, and a non-hydride-forming element, Al. According to previous studies, the interaction of hydrogen with Ti₃Al has been shown to induce destructive hydrogenation, which produces TiH₂ after hydrogenation. The phase separation after hydrogenation limits its reversible hydrogen storage. Recent studies have shown that hydride stability could also be tuned by non-metallic elements. In the present work, we have tried stabilizing the Ti-Al system with the non-metallic element oxygen to suppress destructive hydrogenation. The synthesis of α -Ti[O, Al] starting from TiO₂, Ti, and Al was carried out through the arc melting method. The room-temperature activation of α -Ti[O, Al] was not successful and the activation was performed at 300 °C under 5MPa H₂ pressure. The structural changes after hydrogenation (maximum absorption capacity ~ 3.75 wt%) arose from transformation of α -Ti[O, Al] to a cubic TiH₂. Nonetheless, they recovered their original lattice parameters, which are meaningfully larger than those of α -Ti, after dehydrogenation. The hydrogen storage capacities for various α-Ti[O, Al] compositions generally decrease with increasing oxygen (3.4 and 10 at%) and aluminum content in the alloy. In contrast, for the compositions with a higher oxygen content of 20 at% (Tio.767Alo.033Oo.200 and Tio.790Alo.010Oo.200), the hydrogen storage capacity slightly increases as the Al concentration increases: Ti0.790Al0.010O0.200 (1 at% Al) absorbs 2.91wt% hydrogen whereas Ti0.767Al0.033O0.200 (3.3 at% Al) absorbs 3.04wt% hydrogen. The thermogravimetric analysis profiles show that samples with 20 at.% O release hydrogen at lower temperature even though the major phase after hydrogenation is TiH₂ regardless of the oxygen content. Further analyses are underway to understand the hydrogenation/dehydrogenation mechanism of the Ti-Al-O system and to make it a viable hydrogen storage material.





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Notes

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