



8th International Conference on Nanomaterials Science and Mechanical Engineering University of Aveiro, Portugal July 7-10, 2026

Book of Abstracts



dem
universidade de aveiro
department of mechanical engineering

tema

centre for mechanical
technology and automation



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Anton Paar



**Title**

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Book of Abstracts

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8th International Conference on Nanomaterials Science and Mechanical Engineering

University of Aveiro, Portugal

July 7-10, 2026

(8th ICNMSME-2026)

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

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ICNMSME2026 program

July 7, 2026 (Tuesday)

Auditorium 1		Auditorium 2	
5th International Workshop on “Modern Trends in Energy Research” IWMTER-2026 July 7, 2026, Aveiro, Portugal		International Workshop on High Valued Developments in Photocatalysis [HVDP-2026] The PGK Mandal’s Haribhai V. Desai College of Arts, Science & Commerce (Autonomous) Pune, India Tuesday, 07th July, 2026	
9:00–9:05	Workshop introduction and welcome Address D. Pukazhselvan (Convener IWMTER 2026)	9:30–9:35	Welcome by Dr. Vikram Pandit and Dr. Prakash P. Wadgaonkar
9:05–9:50	Session:1 Chair: Vanessa Graça Plenary Lecture Ihsan Çaha International Iberian Nanotechnology Laboratory, Braga, Portugal Title: “Advanced Transmission Electron Microscopy for Understanding Energy-Related Materials”	9:35–9:40	Inauguration by Principal Dr. Rajendra G. Gurao and Dr. Prakash P. Wadgaonkar
		9:40–10:00	Session Chair: Dr. Vikram Pandit Invited Talk Dr. Gustava Colpani (W2-I1) Community University of Chapecó Region – UNOCHAPECÓ Title: “Heterogeneous Photocatalysis: Fundamentals and Applications”
9:50 - 10:15	Keynote Address D. Pukazhselvan TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal Title: “Ground Analysis: Hydrogen vs Batteries for Vehicular Applications”	10:00–10:20	Invited Talk Dr. Yashpal Rathod (W2-I2) Department of Chemistry, J. M. Patel College of Science, Bhandara (M.S.) INDIA Title: “SYNTHESIS, CHARACTERIZATION AND PHOTOLUMINESCENCE APPLICATION OF SALICYLIC ACID-PHENYL HYDRAZINE FORMALDEHYDE-CHARCOAL COMPOSITE”

10:15–10:35	Session:2 Chair: Francisco Loureiro Invited Talk-1 Aamer Ali Department of Energy, Aalborg University, Denmark <i>Title: “Membrane Technology for Sustainable Energy Transition”</i>	10:20–10:30	Oral Talk Ganesh Dawange (W2-O1) Haribhai V. Desai College, Pune, India <i>Title: “Medicinal Plant-Derived CuO Nanostructures: Visible-Light Photocatalysis and Antibacterial Potential”</i>
10:35–10:55	Invited Talk-2 Sivabalan Maniam Sivasankar Department of Physics, i3N, University of Aveiro, 3810-193, Aveiro, Portugal <i>Title: “Progress in Thin-Film Photovoltaics: Emerging Strategies for High-Efficiency and Scalable Solar Energy Conversion”</i>	10:30–10:40	Oral Talk Sonali Nikam (W2-O2) Research Centre, Department of Chemistry, MG. V. M.S.G.Arts, Science, and Commerce College, Malegaon. (MH), India-423105 <i>Title: “Synthesis of Fe₂O₃-SnO₂ Nanocomposites for Photocatalytic EBT Dye Degradation”</i>
		10:40–10:50	Oral Talk Ganesh Jadhav (W2-O3) Department of Chemistry, The PGK Mandal’s Haribhai V. Desai College of Arts Science and Commerce (Autonomous), Pune-411002, India <i>Title: “Tailored Pr (OH)₃ Nanomaterial for Photocatalysis and Antimicrobial Performance”</i>
10:55–11:15	Invited Talk-3 Parsa Behzad Nazif University of Oviedo, Spain <i>Title: “Parameter Estimation for Digital Twin in Power Electronic Converters”</i>	10:50–11:00	Oral Talk Abhijit Sonone (W2-O4) Modern College, Shivajinagar, Pune, India <i>Title: “Synthesis of Graphene-Based Nanocomposites for Water Purification”</i>

11:15– 11:35	Invited Talk-4 Sathishkumar Duraisamy Centre for Mechanical Technology and Automation (TEMA), Department of Mechanical Engineering, University of Aveiro, Portugal. Title: “Electron Beam Welding of Copper Tubes for Heat Pump Refrigerant Circuits: Process–Property Relationships and Mechanical Performance”	11:00– 11:10	Oral Talk Tushar Patil (W2-O5) Dr. Yusuf Hamied Department of Chemistry, Ramnarain Ruia Autonomous College, Mumbai 400019, India Title: “ZrO₂@S-doped g-C₃N₄ hybrid Nanocomposites for Enhanced Dye Adsorption for MB and MO”
		11:10– 11:20	Oral Talk Sahebrao Dolnar (W2-O6) Dr. Yusuf Hamied Department of Chemistry, Ramnarain Ruia Autonomous College, Mumbai 400019, India Title: “Synergistic effects of α-MnO₂ on the structural, optical and Photocatalytic properties of ZnFe₂O₄”
11:35– 11:45	Session break	11:20– 11:30	Oral Talk Vinícius Tres Orso (W2-O7) Community University of Chapecó Region - UNOCHAPECÓ, Servidão Anjo da Guarda, 295-D, Chapecó, Santa Catarina, Brazil Title: “Development of Titanium Electrodes Modified with Polypyrrole and Niobium for the Photoelectrocatalytic Degradation of Tetracycline and Tramadol”

11:45–12:15	Session:3 Chair: D. Pukazhselvan Invited Talks-5 and 6 Jaykumar Lachure Department of Computer Science and Engineering, Indian Institute of Information Technology (IIIT) Sri City, Chittoor 517646, Andhra Pradesh, India Title: “Quantum-Machine Learning for Discovery of Entropy-Stabilized High-Entropy Alloy Hydrides in Ambient Hydrogen Storage” Jaykumar Lachure / Sagar Lachure Department of Computer Science and Engineering, Indian Institute of Information Technology (IIIT) Sri City, Chittoor 517646, Andhra Pradesh, India Title: “Quantum-ML Discovery of Superionic Proton Ceramic Conductors for 520 Wh/kg Battery Applications”	11:30–11:40	Oral Talk Bhagwan Daphal (W2-O8) Department of Chemistry, Haribhai V. Desai College of Commerce, Arts and Science, Pune-411002, India Title: “Synthesis and Characterization of Polyaniline Vanadium Pentoxide nanocomposite for Photocatalytic Degradation of Organic Pollutants”
		11:40–11:50	Oral Talk Priyanka Bhalerao (W2-O9) Dr. T. R. Ingle Research Laboratory, Department of Chemistry, S. P. College, Pune–30, India Title: “Controlled Hydrothermal Synthesis of CoS₂ Microspheres toward Multifunctional Energy and Biological Applications”
		11:50–12:00	Vote of Thanks/Concluding remarks
12:15–12:35	Invited Talk-7 Carlos O Amorim Department of Physics and i3N, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal Title: “Impact of Dilute Ag Distribution on Sequentially Sputtered Cu(In,Ga)(Se,S)₂ Solar Cell Performance”		

12:35– 12:55	Invited Talk-8 Deepa M. J Department of Chemistry, University of Kerala, Kariavattom campus, Thiruvananthapuram. 69558, India Title: “Interface-Engineered WO₃/Co₃O₄ Heterostructure in NiCoP Alloy Coating for Efficient Alkaline Hydrogen Evolution Reaction”	
12:55– 13:15	Invited Talk-9 Francisco J. A. Loureiro TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal Title: “Mixed ionic and electronic conductors: fundamentals and optimisation strategies”	
13:15– 13:25	Vote of Thanks/Concluding remarks D. Pukazhselvan (convener) Francisco Loureiro (Co-convener)	
13:25– 14:00	Lunch	
6th Workshop on New Challenges of Bionanomaterials: Science, Technology, Application, University of Aveiro, Portugal, July 7, 2026		
14:00– 14:05	WELCOME ADDRESS Dr. Igor Bdikin, Dr. Gil Gonçalves	



14:05– 15:00	CHAIR: Dr. Gil Gonçalves Plenary Lecture Dr. Igor Bdikin Atomic Force Microscopy Methods for Characterization of Organic and Biological Low-dimensional Structures <i>Institute of Solid State Physics, University of Latvia, Kengaraga iela 8, LV-1063 Riga, Latvia</i>	
15:00– 15:20	Plenary Lecture Prof. Dr. Carla I. M. Santos Exploring the conjugation of carbon based materials with tetrapyrrolic macrocycles: New Applications and Challenges <i>LAQV-REQUIMTE, Department of Chemistry of University of Aveiro, 3810-193 Aveiro, Portugal</i> <i>Centro de Química Estrutural, Institute of Molecular Science and Departamento de Engenharia Química, Instituto Superior Técnico, Universidade de Lisboa, 1049-001 Lisboa, Portugal</i>	
15:20– 15:25	Vote of Thanks/Concluding remarks	

July 8, 2026 (Wednesday)

8th International Conference on Nanomaterials Science and Mechanical Engineering ICNMSME-2026	
9:00-9:10	WELCOME ADDRESS: Prof. Dr. Robertt Angelo Fontes Valente (UA, Portugal), Prof. Dr. Vítor António Ferreira da Costa (UA, Portugal), Prof. Dr. António Manuel de Bastos Pereira (UA, Portugal), Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques (UA, Portugal), Dr. Duncan Paul Fagg (UA, Portugal), Dr. Igor Bdikin (UA, Portugal), Dr. Gil Alberto Batista Gonçalves (UA, Portugal), Natália Barroca (UA, Portugal), Francisco Loureiro (UA, Portugal), Laura Holz (UA, Portugal), Vanessa Cristina Diniz da Graça (UA, Portugal)
9:10-9:30	CHAIR: Dr. Natália Barroca Session: Optical Materials Keynote talk Dr. Suresh Kumar Jakka (14) Advanced Chalcogenide and Tellurite Glasses for Mid-Infrared Photonics, Sensing, and Light Conversion <i>I3n & Physics Department, University of Aveiro, Aveiro 3810-193, Portugal</i>
9:30-10:30	Session: Biomaterials Plenary Lecture Prof. Dr. Robert C. Pullara Sustainable scaffolds: 3D printed bioceramic bone scaffolds for biomedical applications obtained from valorised fish wastes for the first time <i>Department of Molecular Science and Nanosystems (DSMN), Ca' Foscari University of Venice, Via Torino 155, 30172 Venezia Mestre, Venice (VE), Italy</i>
10:30-10:50	Coffee break
10:50-11:10	Session: Thin Films Keynote talk Prof. Dr. Aleksandr Bagmut (12) Crystallization of amorphous Yb₂O₂S films <i>National Technical University "Kharkiv Polytechnic Institute", Kharkiv, Ukraine</i>
11:10-11:30	Session: Thin Films Keynote talk Dr. Pavel Zelenovskii (19) Piezoelectric polycrystalline thin films of dileucine for energy harvesting <i>Department of Physics and CICECO – Aveiro Institute of Materials, University of Aveiro, Portugal</i>

Auditorium 1		Auditorium 2	
	CHAIR: Dr. Natália Barroca		CHAIR: Dr. Indrani Coondoo
11:30-11:45	Session: Thin Films Dr. Hameed Ullah (O10) Growth, interfacial reactions, and properties of diamond and BDD thin films grown by MPCVD on Nb-coated silicon <i>Chair of Surface and Materials Technology, Institute of Materials Engineering, University of Siegen, Germany</i>	11:30-11:45	Session: Polymer films Zeynep Ziyade ÖZACAR (O24) pH-Sensitive and Antioxidant PVA–CMC Films Incorporating Eggplant Peel Extract <i>Sakarya University, Institute of Natural Sciences, Department of Chemistry, Türkiye</i>
11:45-12:00	Session: Thin Films Ama Hettiarachchi (O47) Comparative Study of N₂ and H₂S Annealing on Grain Growth and Surface Morphology of CZTS Thin Films <i>Department of Physics and Electronics, University of Kelaniya, Sri Lanka</i>	11:45-12:00	Session: Surface Engineering Kinani Ihsane (O60) Engineering of new biobased hydrophobic polymers for slow release fertilizer: Formulation and agronomic assessment <i>Faculté des Sciences et Techniques de Mohammedia, Université Hassan II de Casablanca, Maroc</i>
12:00-12:15	Session: Thin Films Dr. Shiva. L. Udachan (O32) Thin-Film Deposition Techniques <i>Department of Physics, School of Advanced Sciences, KLE Technological University, Hubballi-India</i>	12:00-12:15	Session: Nanotechnology Dr. Jéniffer Gómez (O50) Engineering solar-driven systems for sustainable water treatment through low-dimensional materials <i>CICA-Centro Interdisciplinar de Química e Biología, Universidade da Coruña, As Carballeiras, Spain</i>
12:15-12:30	Session: Thin Films Dr. Deepa K G (O46) Development of a Self-Powered CuInSe₂/Si Photodetector <i>Department of Physics, University of Kerala, Thiruvananthapuram, India</i>	12:15-12:30	Session: Nanotechnology Hind Asserghine (O82) Tailoring Spin Textures in Two-Dimensional Chromium Nitride via Half-Halogenation <i>LPHE-MS, Faculty of Science, Mohammed V University in Rabat, Morocco</i>
12:30-12:45	Session: Thin Films NDIBI Brenton Hubert (O16) Preparation of bioplastic films from <i>Abelmoschus esculentus</i> by Microwave Assisted Extraction: Influence of microwaving time on the film's properties <i>University of Yaounde, Cameroon</i>	12:30-12:45	Session: Nanotechnology Dr. Shah Rukh Abbas (O12) Peptide functionalized phase convertible targeted nanodroplets for ultrasound triggered drug release across Blood Brain Barrier <i>Biosensors and Therapeutics Lab, Atta ur Rahman School of Applied Biosciences (ASAB), National University of Sciences and Technology (NUST), Pakistan</i>
12:45-14:00	Lunch		

CHAIRS: Dr. Gil Gonçalves, Dr. Francisco Loureiro		Session: Nanotechnology	
Plenary Lecture			
14:00-14:40	Prof. Dr Senentxu Lanceros-Méndez Polymer based nano-composite membranes for energy and environmental applications <i>BCMaterials, UPV/EHU Science Park, Leioa, Spain</i> <i>Ikerbasque, Basque Foundation for Science, Bilbao, Spain</i> <i>Physics Centre of Minho and Porto Universities (CF-UM-UP) and Laboratory of Physics for Materials and Emergent Technologies (LapMET), University of Minho Braga, Portugal</i>		
		Session: Nanotechnology	
Plenary Lecture			
14:40-15:10	Dr. Gil Gonçalves Carbon-Based Nanocomposites at the Crossroads of Healthcare, Environment, and Energy <i>Centre for Mechanical Technology and Automation (TEMA), University of Aveiro, Aveiro 3810-193, Portugal</i>		
		Session: Micro / Nano Materials	
Keynote talk			
15:10-15:30	Dr. Zhi Jiang (I10) Synthesis of Highly Crystalline Microdiamonds via Nano-Silicon Assisted Liquid Metal CVD <i>Centre for Mechanical Technology and Automation (TEMA), University of Aveiro, Aveiro 3810-193, Portugal</i>		
15:30-15:45	Coffee break		
Auditorium 1		Auditorium 2	
15:45-16:00	CHAIRS: Dr. Francisco Loureiro, Dr. Zhi Jiang Session: Low Dimension Structures Dr. Manuel Vázquez Sulleiro (O51) Covalent Engineering of Transition Metal Dichalcogenides: From Molecular Design to Hybrid Heterostructures <i>Centro Interdisciplinar de Química e Biología (CICA), Universidade da Coruña, Spain</i>	15:45-16:00	CHAIRS: Dr. Pavani Krishnapuram, Dr. Martina Kocijan Session: Modelling Properties Materials Dr. Merwan Behar (O48) Piezoelectric and spin effects on the vibration behavior of spinning SWZnONTs <i>MECACOMP Laboratory, Department of Mechanical Engineering, Faculty of Technology, Algeria</i>
16:00-16:15	Session: Low Dimension Structures Prof. Dr. Andrii Goriachko (O52) Nanometer Scale 2D Structures in Cerium + Oxygen Submonolayer Films on Mo(112) Surface: Experiment + Theory <i>Institute of Physics, National Academy of Sciences of Ukraine, Kyiv, Ukraine</i>	16:00-16:15	Session: Modelling Properties Materials Dr. Neda Mousavi (O1) Tensile Mechanical Properties of Goldene Nanotubes: A molecular Dynamics Simulation <i>Department of Physics, Faculty of Science, University of Zanjan, Iran</i>
16:15-16:30	Session: Low Dimension Structures Dr. Ahmed Lamine Aouinat (O56) Gyroscopic Effects in Rotating Functionally Graded Nanotubes: An Exact Analytical Study <i>Mechanical Engineering, University of Tlemcen, Algeria</i>	16:15-16:30	Session: New Methods of Modeling Properties Materials Justyna Niewiadomska-Kaplar (O20) High-, low-, and zero-spin compounds and structural variety' of 3d metals <i>Tab edizioni, Roma, Italy</i>

16:30-16:45	Session: Micro / Nano Materials Dr. Ahmed Lamine Aouinat (O57) Influence of Material Gradient Index and Composition on the Vibrational and Dynamic Properties of CNT/SiCNT Functionally Graded Nanotubes <i>MECACOMP Laboratory, Dept. of Mechanical Engineering, University of Tlemcen, Algeria</i>	16:30-16:45	Session: Nanotechnology Dr. Rafael Omar Torres Mendiet (O8) Engineering Nested NiPd Nanostructures by Reactive Laser Ablation for Advanced Selective Hydrogenation Catalysis <i>Department of Chemical Sciences, University of Padua, Italy</i>
16:45-17:00	Session: Materials Science Dr. Mostafa Sadeghian (O15) What role does artificial intelligence play in modern mechanical and material engineering? <i>Faculty of Mechanical Engineering and Design, Kaunas University of Technology, Kaunas, Lithuania</i>	16:45-17:00	Session: Nanotechnology Prof. Dr. Skander Ktifa (O13) High performance of Ag/AlN/Si Schottky diode: Study of the DC sputtering power effect on its electrical properties <i>School of Physics, University College Dublin, Ireland</i> <i>Laboratory of Photovoltaic, Energy Research and Technology Center, Technopole of Borj-Cedria, Tunisia</i>
17:00-17:15	Session: Mechanical Engineering Nawal Ashraf (O53) Optimizing Process Parameters for Nanomachining of Lithium Niobate <i>School of Physics, University College Dublin, Ireland</i>	17:00-17:15	Session: Nanotechnology Soheil Saeedi (O80) Preparation and Characterization of P-123 Stabilized Functionalized Multi-Walled Carbon Nanotube Particles <i>Sakarya University, Faculty of Science, Department of Chemistry, Sakarya, Türkiye</i>
17:15-17:30	Session: Nanocomposite Tushar Patil (O36) ZrO₂@S-doped g-C₃N₄ hybrid Nanocomposites for Enhanced Dye Adsorption for MB and MO <i>Dr. Yusuf Hamied Department of Chemistry, Ramnarain Ruia Autonomous College, Mumbai, India</i>	17:15-17:30	Session: Nanotechnology Meryem Uzun (O81) Photocatalytic Degradation of Methylene Blue Using TiO₂/Carboxymethyl Cellulose Hydrogel Films <i>Sakarya University, Institute of Natural Sciences, Department of Chemistry, Türkiye</i>

July 9, 2026 (Thursday)

8th International Conference on Nanomaterials Science and Mechanical Engineering ICNMSME-2026				
9:00-9:20	CHAIRS: Dr. D. Pukazhselvan, Dr. Francisco J. A. Loureiro Session: Hydrogen and Fuel Cell Science <i>Keynote talk</i> Dr. Vanessa C.D. Graça (I7) Cubic Niobium Oxynitride: A Novel Electrode Material for Proton Ceramic Membrane Reactors <i>TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal</i>			
	Session: Hydrogen and Fuel Cell Science <i>Keynote talk</i> Dr. Francisco J. A. Loureiro (I8) Yttrium-doped barium stannate: A carbonation-resistant perovskite anode component for proton ceramic electrochemical cells <i>TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal</i>			
9:40-10:20	Session: Hydrogen and Fuel Cell Science <i>Plenary Lecture</i> Dr. D. Pukazhselvan Screening the hydrogen storage materials for vehicular applications <i>TEMA – Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal</i>			
10:20-10:30	Coffee break			
Auditorium 1		Auditorium 2		
10:30-10:45	CHAIRS: Dr. D. Pukazhselvan, Dr. Francisco J. A. Loureiro Session: Hydrogen and Fuel Cell Science Dr. Morena Brito de Farias (O69) Optimization of cobalt-free mixed ionic-electronic conducting electrodes for solid oxide cells <i>Materials Science and Engineering Postgraduate Program – PPGCEM, Federal University of Rio Grande do Norte, Brazil</i>		10:30-10:45	CHAIR: Dr. André Girão Session: Biomaterials Florian GILSOUL (O63) Relaxation dynamics of poly(lactic-co-glycolic) acid nanocomposites <i>Univ Rouen Normandie, INSA Rouen Normandie, CNRS, Normandie Univ, France</i>

10:45-11:00	Session: Hydrogen and Fuel Cell Science Dr. Alina Kozhukhova (O3) Catalyst and support engineering for next-generation passive autocatalytic recombiners <i>Hydrogen South Africa (HySA) Infrastructure, Faculty of Engineering, North-West University, Potchefstroom, South Africa</i>	10:45-11:00	Session: Biomaterials Sanaa Oumnas (O44) Structure and relaxation dynamics in electrospun polylactide nanofibers: influence of the molecular weight <i>Univ Rouen Normandie, INSA Rouen Normandie, CNRS, Normandie Univ, France</i>
11:00-11:15	Session: New Materials and Advanced Materials Himashee Naranpanawa (O54) Preliminary Study on Thermal Quenching-Induced Exfoliation of Vein Graphite using HCl Acid Medium <i>National Center for Advanced Battery Research, National Institute of Fundamental Studies, Kandy, Sri Lanka</i>	11:00-11:15	Session: New Materials and Advanced Materials Dr. Mohamad Danial Shafiq (O14) Structure-Tribology Correlations of Imidazolium- and Phosphonium-Based Green Dispersants for Carbon Stabilization in Oil <i>School of Materials and Mineral Resources Engineering, Universiti Sains Malaysia, Penang, Malaysia</i>
11:15-11:30	Session: Hydrogen and Fuel Cell Science Dr. Allan J. M. Araújo (O70) What catalysts can enable hydrocarbon-fuelled protonic ceramic cells? <i>TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal</i>	11:15-11:30	Session: Biomaterials Prof. Dr. Goutam Thakur (O19) Impact of pH, freezing temperature, and crosslinking on the transport of diclofenac sodium from freeze-dried chitosan scaffolds <i>School of Electrical Engineering, Manipal Institute of Technology, Karnataka, India</i>
11:30-11:45	Session: Hydrogen and Fuel Cell Science Dr. Daniela V. Lopes (O7) Electrochemical evaluation of Ni-based composite electrodes for alkaline hydrogen evolution <i>CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Portugal</i>	11:30-11:45	Session: Biomaterials Muhammet Kamil Kerim (O45) Corchorus olitorius-Loaded PVA/PVP Hydrogels for Wound Dressing Applications <i>Sakarya University, Institute of Natural Sciences, Department of Biomedical Engineering, Turkiye</i>
11:45-12:00	Session: Composites Prof. Dr. Xueying ZHANG (O34) One-Pot Synthesis of Metal Nanocomposites/Graphene through Pulsed Wire Discharge <i>School of Mechatronical Engineering, Beijing Institute of Technology, Beijing, China</i>	11:45-12:00	Session: Biomaterials Prof. Dr. Münteza ÖZSOY (O35) Synthesis and Characterization of Amoxicillin-Loaded Beta-Cyclodextrin Nanocarriers and Assessment of the Influence of Pectin Coating on Controlled Drug Release <i>Department of Pharmaceutical Toxicology, Faculty of Pharmacy, Kocaeli Healthy and Technology University, Turkey</i>

12:00-12:15	Session: Hydrogen and Fuel Cell Science Prof. Dr. Azzam Alfarraj (O22) Graph-Based Machine Learning Framework for Predicting Hydrogen Storage Capacity in Metal-Organic Frameworks <i>Department of Mathematics and Interdisciplinary Center of Smart Mobility and Logistics, King Fahd University of Petroleum & Minerals, Dhahran, Saudi Arabia</i>	12:00-12:15	Session: Biomaterials Dr. Djahida SIDANE (O49) Modification of the Physical and Chemical Properties of Biomaterials Derived from Sol-Gel Technology <i>Université de Bejaia, Faculté de Technologie, Laboratoire de Génie de l'Environnement (LGE), Algeria</i>
12:15-12:30	Session: Composites Dr. Mohsan Nawaz (O11) Micronutrient-loaded Chitosan-Polyethylene Glycol Nanocomposite Coatings: Synthesis, Characterization, and Field Evaluation for Improved Wheat Germination and Productivity <i>Department of Chemistry Hazara University, Mansehra, Pakistan</i>	12:15-12:30	Session: Nanocomposite Omkar Malusare (O43) g-C₃N₄ Nanocomposites for Enhanced Dye Adsorption for MB and MO <i>Haribhai V. Desai College, Pune, India</i>
12:30-12:45	Session: Hydrogen and Fuel Cell Science Alfredo Luemba (O73) Phase Stability of Ruddlesden-Popper Ba₂SnO₄ under reducing atmosphere to Proton Ceramic Cells <i>TEMA – Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal</i>	12:30-12:45	Session: Metal-organic frameworks Mahsa Heidarnesjad (O33) Synthesis, Characterization, and Drug Release Profile of Cerium based Metal Organic Frameworks Loaded with Quercetin for Cancer Treatment <i>Sakarya University, Institute of Natural Sciences, Department of Chemistry, Turkiye</i>
12:45-14:00	Lunch		
14:00-14:20	CHAIRS: Dr. Andrei Kovalevsky, Dr. Suresh Kumar Jakka Session: Optical Materials Keynote talk Dr. Pavani Krishnapuram (I6) Spectroscopic investigations of Laser Floating Zone grown Lanthanum Aluminate crystals <i>i3N & Department of Physics, University of Aveiro, Aveiro 3810-193, Portugal</i>		
14:20-14:40	Session: Company presentation Dr Ana M. Fuentes-Caparrós (C1) Nanomechanical Testing of Heterogeneous and Advanced Materials <i>Anton Paar TriTec SA, Les Vernets 6, 2035 Corcelles-Cormondrèche (Neuchatel), Switzerland</i>		

Auditorium 1		Auditorium 2	
	CHAIRS: Dr. Andrei Kovalevsky, Dr. Suresh Kumar Jakka Session: New Materials and Advanced Materials Miljana Dukić (O21) Visible-Light-Active ZrO₂ Interfacial Charge-Transfer Complexes for Photocatalytic Hydrogen Evolution <i>Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Centre of Excellence for Photoconversion, Belgrade, Serbia</i>		CHAIR: Prof. Dr. Neeraj Panwar Session: Biomaterials Dr. Ashish Chalana (O5) In-Situ Hydrothermal Design of Metal Chalcogenides Decorated 2D Materials Nanocomposites as Artificial Peroxidase Enzyme <i>Department of Chemistry & Biochemistry, Sharda School of Engineering & Science, Sharda University, India</i>
14:40-14:55		14:40-14:55	
	Session: New Materials and Advanced Materials Prof. Dr. Soner ÇAKAR (O37) Electrochemical sensing of sunset yellow with GCE/V2O5-rGO nanocomposite electrode <i>Sakarya University, Biomaterials, Energy, Photocatalysis, Enzyme Technology, Nano & Advanced Materials, Additive Manufacturing, Environmental Applications and Sustainability Research & Development Group (BIOENAMS R&D Group), Sakarya, Türkiye</i>		Session: Biomaterials Hajar OUSGHIR (O68) Development of Standard Cosmetic Formulations as Reference Prototypes for Future Eco-Friendly Bioformulations from Moroccan Biomass By-Products <i>Laboratory of biotechnologies, agri-food, materials and environment, URAC 24, Faculty of Science and Technology, Hassan II University, Casablanca, Morocco</i>
14:55-15:10		14:55-15:10	
	Session: New Materials and Advanced Materials Prof. Dr. Soner ÇAKAR (O38) Development of MIL-101(Fe)/TiO₂ photoanode for dye sensitized solar cells <i>Sakarya University, Biomaterials, Energy, Photocatalysis, Enzyme Technology, Nano & Advanced Materials, Additive Manufacturing, Environmental Applications and Sustainability Research & Development Group (BIOENAMS R&D Group), Sakarya, Türkiye</i>		Session: Biomaterials Bartosz Klebowski (O71) Proton therapy assisted by palladium nanospheres (Pd Sph) and palladium nanocubes (Pd Cub) – in vitro studies <i>Institute of Nuclear Physics Polish Academy of Sciences, Krakow, Poland</i>
15:10-15:25		15:10-15:25	
	Session: New Materials and Advanced Materials Prof. Dr. Lynda Djoudi (O39) Phase Evolution and Optical Properties of Cr/Al Co-Doped BiFeO₃ Nanoparticles Synthesized via a Sol-Gel Route <i>Laboratory of Molecular Chemistry and Environment, University Mohamed Khider of Biskra, Algeria</i>		Session: Biomaterials Eliz ELYILDIRIM (O79) Investigation of the influence of titanium dioxide (TiO₂) on Carboxymethyl Cellulose (CMC) based hydrogels <i>Sakarya University, Biomedical, Magnetic and Semiconductor Materials Research Center (BIMAS-RC), Sakarya, Türkiye</i>
15:25-15:40		15:25-15:40	

15:40-15:55	Session: New Materials and Advanced Materials Esra ÇAKAR (O40) BiVO₄/MWCNT composite electrodes for photoelectrochemical carmoisine detection <i>Sakarya University, Faculty of Science, Department of Chemistry, Sakarya, Türkiye</i>	15:40-15:55	Session: Eco-friendly materials Prof. Smita V. Deore (O74) An Efficient and Sustainable Metal-Free Synthesis of Highly Substituted Piperidines Derivatives under Ultrasound Irradiation <i>Department of Chemistry, MES's Nowrosjee Wadia College, Pune, India</i>
15:55-16:10	Session: Composites Oluwasegun Emmanuel Ojodun (O9) Mechanistic Insights into the Structural, Electrochemical, and Charge-Storage Behavior of CNT@NiO Electrodes for High Capacitance and Durable Supercapacitors <i>Department of Mechanical Engineering Science, University of Johannesburg, Johannesburg, South Africa</i>	15:55-16:10	Session: Electrocatalysts Priyanka Bhalerao (O67) Controlled Hydrothermal Growth of Hollow CoS₂ Microspheres as High-Performance HER electrocatalysts <i>Dr. T. R. Ingle Research Laboratory, Department of Chemistry, S. P. College, Pune, India</i>
16:10-16:30	Coffee break		
16:30-16:45	Session: New Materials and Advanced Materials Dr. Andreea Elena Maftai (O17) Spiropyran-coated magnetite used for pollutant removal <i>Department of Exact and Natural Sciences, Institute of Interdisciplinary Research, Alexandru Ioan Cuza University of Iași, Romania</i>	16:30-16:45	Session: Environmental Friendly Materials Dr. Alyona Yanevich (O18) MOF- and ZIF-Integrated Cryogels as Monolithic Adsorbents for Water Purification: Synthesis, Characterization, and Sorption Performance <i>Department of Chemistry and Chemical Technology, Manash Kozybayev North Kazakhstan University, Petropavlovsk, Kazakhstan</i>
16:45-17:00	Session: Composites Oumayma Bouhajeb (O25) Ag, Ag₂O, and Ag-Ag₂O modified BaTiO₃/ZnO Heterostructures for Enhanced Visible-Light Photocatalysis <i>Laboratoire de Chimie Minérale Appliquée (LCMA) LR19ES02, Faculté des Sciences de Tunis, Université Tunis El Manar. Campus Universitaire Farhat HACHED, Tunisie</i>	16:45-17:00	Session: Environmental Friendly Materials Yousra Belayachi (O58) Eco-Friendly Biopolymer-Based Hydrogels for Controlled Water Release in Sustainable Agriculture <i>Laboratory of biotechnologies, agrifood, materials and environment, URAC 24, Faculty of Science and Technology, Hassan II University, Casablanca, Morocco</i>

17:00-17:15	Session: Composites Oumayma Bouhajeb (O26) Effect of silver on BaTiO₃/ZnO based nanocomposites for antibacterial application <i>Laboratoire de Chimie Minérale Appliquée (LCMA) LR19ES02, Faculté des Sciences de Tunis, Université Tunis El Manar. Campus Universitaire Farhat HACHED, Tunisie</i>	17:00-17:15	Session: Environmental Friendly Materials Beatriz Valadares (O55) Magnetic TiO₂/Carbon Quantum Dots nanocomposites as sustainable photocatalysts for antibiotic removal from water <i>Department of Chemistry, University of Aveiro, Portugal</i>
17:15-17:30	Session: Ceramics Mehdi Hedayati (O61) Ni-Assisted Densification and Electrochemical Characterization of BaCe_{0.7}Zr_{0.1}Y_{0.1}Yb_{0.1}O_{3-δ} Proton-Conducting Ceramics <i>CICECO-Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Portugal</i>	17:15-17:30	Session: New Materials and Advanced Materials Luís Miguel Gomes Ferreira (O76) Incorporation of graphene oxide in concrete: from car batteries to reinforced construction materials <i>Chemistry Centre of University of Minho, Braga, Portugal</i>
17:30-18:30	CHAIRS: Dr. Igor Bdikin, Dr. Suresh Kumar Jakka Poster session, July 9, 2026 (Thursday), 17:30-18:30		

July 10, 2026 (Friday)

8th International Conference on Nanomaterials Science and Mechanical Engineering ICNMSME-2026	
CHAIRS: Dr. Andrei Kovalevsky, Dr. Vanessa Graça	
9:00-9:20	Session: Composites Keynote talk Prof. Dr. Neeraj Panwar (I5) Bias-voltage Induced Transition from Capacitive-coupled to Purely Resistive Switching Behaviour in Ag/PVA-Graphene oxide/FTO Devices <i>Department of Physics, Chaudhary Charan Singh University, India</i>
9:20-9:40	Session: Optical/Electronic/Magnetic Materials Keynote talk Dr. Venkata Eskilla (I3) Engineering Functional Cobalt Oxide Perovskites for Advanced Electronics <i>i3N-Aveiro, Department of Physics, University of Avrio, 3810-193, Portugal</i>
9:40-10:00	Session: Ceramics Keynote talk Dr. Gunnar Suchaneck (I1) Impact of Antisite Disorder on the Resistivity of Sr₂FeMoO₆ Ceramics <i>Department of Physics, University of Kerala, Thiruvananthapuram, India Institute of Solid-State Electronics, TU Dresden, Germany</i>
10:00-10:15	Session: Composite and Building Materials Wahyudin (O65) Finite Volume Method in Heat Transfer Process in Paraffin, Zeolite and Ice Pack Based Brick Composites <i>Department of Mechanical Engineering, Universitas Muhammadiyah Pontianak, Indonesia</i>
10:15-10:30	Coffee break
10:30-10:45	Session: Composite and Building Materials Yeyen Dea Arisandi (O64) Analysis of Two-Dimensional and Three-Dimensional Heat Conduction in Composite Thermal Storage Materials <i>Department of Mechanical Engineering, Universitas Muhammadiyah Pontianak, Indonesia</i>

10:45-11:00	Session: Composite and Building Materials Indra Ramadhan (O66) Experimental Study of Energy-Efficient Wall Using Hybrid PCM (Paraffin, Ice Pack, and Zeolite) Under Tropical Climate Conditions <i>Department of Mechanical Engineering, Universitas Muhammadiyah Pontianak, Indonesia</i>
11:00-11:15	Session: Photocatalysis Karishma Suryawanshi (O29) Visible-Light Photocatalytic Degradation of Rhodamine 6G Using Thiourea-Derived Graphitic Carbon Nitride <i>Haribhai V. Desai College, Pune, India</i>
11:15-11:30	Session: Photocatalysis Ganesh Dawange (O28) Synthesis of green copper oxide photocatalysts for use in photocatalysis and antibacterial agents by means of plant extract <i>Haribhai V. Desai College, Pune, Maharashtra, India</i>
11:30-11:45	Session: Photocatalysis Bhagwan Daphal (O42) Synthesis and Characterization of Polyaniline for Photocatalytic Degradation of Organic Pollutants <i>Department of Chemistry, Haribhai V. Desai College of Commerce, Arts and Science, Pune, India</i>
11:45-12:00	Session: Photocatalysis Prof. Abhijeet Sonone (O72) Graphene-Based Ternary Nanocomposites for Water Purification Applications <i>Modern College, Shivajinagar, Pune, India</i>
12:00-12:15	Session: Photocatalysis Bhagyashree Gogawale (O30) Urea-Derived Graphitic Carbon Nitride as a Catalyst for NaBH₄-Assisted Dye Reduction in Aqueous Medium <i>Haribhai V. Desai College, Pune, India</i>
12:30-14:00	Lunch
14:00-14:15	CHAIRS: Dr. Venkata Eskilla, Dr. Martina Kocijan Session: Photocatalysis Sakshi Salunke (O31) Melamine-Derived Graphitic Carbon Nitride for Visible-Light Degradation of Chlorophenol Pollutants <i>Haribhai V. Desai College, Pune, India</i>

14:15-14:30	Session: 2D photocatalyst Santosh Dhavale (O41) Transition Metal Dichalcogenides for Visible-Light Photocatalytic Degradation of Organic Pollutants - Background, Synthesis, Characterization, and Mechanistic Insights <i>Modern College of Arts, Science and Commerce, Shivajinagar, Pune, India</i>
14:30-14:45	Session: Photochromic materials Cătălina-Nicoleta Basoc (O23) Novel photochromic materials for micropollutants removal <i>Department of Exact and Natural Sciences, Institute of Interdisciplinary Research, Alexandru Ioan Cuza University of Iasi, Romania</i>
14:45-15:00	Session: Sensor Materials Dr. Muhammad Nasir (O6) Smart Hybrid Nanozymes for Portable and Reagentless Colorimetric Sensing and Point of Care Detection <i>Interdisciplinary Research Centre in Biomedical Materials (IRCBM), COMSATS University Islamabad, Lahore Campus, 1.5 Km Defence Road, Off Raiwind Road, Lahore, Punjab, Pakistan</i>
15:00-15:15	Session: Sensor Materials Tomás Barros (O75) Influence of Cu:Ag Composition on Ionic Release and Longevity of Wearable Dry Electrodes <i>Chemistry Centre, University of Minho, Gualtar, Braga, Portugal</i>
15:15-15:45	Coffee break
15:45-16:00	Session: Sensor Materials Dr. Cláudia Lopes (O78) Nanostructured Flexible Dry-Electrodes for Personalized and Preventive Digital Healthcare <i>TEMA - Nanotechnology Research Group, Mechanical Engineering Department, University of Aveiro, Portugal</i>
16:00-16:15	Session: Thin Films Dr. Hassane MES-ADI (O27) Atomistic analysis of indentation-induced deformation in Nb thin films <i>Laboratoire d'ingénierie des Procédés, Informatique et Mathématiques, Ecole Nationale des Sciences Appliquées Khouribga, Université Sultan Moulay Slimane - Beni Mellal, Khouribga, Morocco</i>
16:15-16:45	Session: Thin Films Ana Camarinha (O77) Tailoring the Microstructure and Electrical Properties of Ti-Au Thin Films via Glancing Angle Deposition for Dry Electrode Applications <i>Faculty of Engineering of University of Porto, Portugal</i>
16:45-17:00	Session: Thin Films Dr. Soukaina BENYAMANE (O59) Formulation of Biopolymer-Based pH-Responsive Indicator Films for Smart Food Packaging <i>Laboratory of biotechnologies, agrifood, materials and environment, URAC 24, Faculty of Science and Technology, Hassan II University, Casablanca, Morocco</i>
17:00-17:15	Session: Composites Diogo Sousa (O62) Approaches for recovery and reuse of nickel from end-of-life high-temperature fuel cells <i>CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Portugal</i>

17:15-17:30	Session: Metal alloy Materials Adélio Fumo (O2) Sustainable production of Fe-Ni alloy from nickel iron oxide by electroreduction in strongly alkaline suspensions <i>Department of Materials and Ceramic Engineering, CICECO – Aveiro Institute of Materials, University of Aveiro, Portugal</i>
17:30-17:45	Conference Closing Ceremony

Poster session, July 9, 2026 (Thursday), 17:30-18:30

P1	Surface effects on mode-I crack tip fields: A finite element simulations Kamel Yaya <i>University of Bejaia, Faculty of Technology, Laboratoire de Mécanique, Matériaux & Energétique (L2ME), 06000 Bejaia, Algeria</i>
P2	Tuning Crystal Facets of BiVO₄ for Enhanced Charge Separation Tayebah Sharifi, Dmitrii Deev, Marko Štrok, Aleš Lapanje <i>Jožef Stefan Institute, Jamova cesta 39, 1000, Ljubljana, Slovenia</i>
P3	The Nanoscience Dalmatian: Metal Decorated Titanium Dioxide Nanoparticles via Spark Ablation Mariia Becker, Benjamin Gfeller, Markus Kalberer <i>University of Basel, Department of Environmental Sciences, Klingelbergstrasse 27, 4056 Basel, Switzerland</i>
P4	Investigation of physical properties of new Silicon Telluride compounds from First-Principles Calculations H. Krarcha, A. Ferroudj <i>Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Centre of Excellence for Photoconversion, P.O. Box 522, 11001, Belgrade, Serbia</i> <i>Lrprim laboratory Department of physics, Faculty of material sciences, University Batna 1.05000, Algeria; Earth science & Universe institute , University Batna2.05002, Algeria; Laboratoire d'Etudes Physico-Chimique des Matériaux (L.E.P.C.M) Batna 1 University, Algeria</i>
P5	Overview of binary noble metal-rare earth compounds A.Ferroudj, H. Krarcha, A.B.Ferroudj <i>Department of physics, Faculty of material sciences, University batna1.05000.Algeria; Lrprim laboratory Department of physics, Faculty of material sciences, University batna1.05000. Algeria; Earth science & Universe institute , University batna2.05002.Algeria; Laboratoire d'Etudes Physico-Chimique des Matériaux (L.E.P.C.M)Batna 1 University, Algeria</i>
P6	Designing Materials with Optoelectronic and Photovoltaic Properties as Potential Dopant-free Hole Transport Materials for Advanced PSCs Javed Iqbal <i>Department of Chemistry, College of Sciece, University of Bahrain, Kingdom of Bahrain</i>
P7	Chiral and Entropic Interactions in Self-Assembly of Cellulose Nanocrystals (SCNCs) into Optically Active liquid crystals Rachel Yerushalmi-Rozen <i>Dept. of Chem. Eng. Ben-Gurion University of the Negev, Israel</i>

P8	Tolerance synthesis in mechanical assemblies using Monte Carlo simulation Said Boutahari, Mouhssine Chahbouni, Anass El-Qemary, Ikram Kabbouri <i>TSI laboratory, Higher school of technology, Sidi Mohammed Ben Abdellah University Imouzzet street, BP 2427 (30000), Fez, Morocco</i>
P9	Magnetron-sputtered AZO thin films on 3D-printed substrates for sEMG and SmO₂ sensing André S. Macedo, Filipe Vaz, Cláudia Lopes <i>Physics Center of Minho and Porto Universities (CF-UM-UP), University of Minho, Campus de Azurém, 4800-058, Guimarães, Portugal; LaPMET–Laboratory of Physics for Materials and Emergent Technologies, University of Minho, Braga, Portugal; TEMA- Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal; LASI - Intelligent Systems Associate Laboratory, 4800-058 Guimarães, Portugal</i>
P10	Deformations in nanocomposites of multiwalled carbon nanotubes and polymers, SiO₂ A. P. Onanko, L. V. Kuzmych, Y. A. Onanko, G. V. Voropai, S. A. Kuzmych, O. P. Dmytrenko, M. P. Kulish, L. Y. Matzui, A. P. Naumenko, T. M. Pinchuk-Rugal, A. G. Rugal, O. L. Pavlenko, V. V. Kuryliuk, A. M. Kuryliuk, L. I. Kurochka, P. P. Ilyin <i>Taras Shevchenko National University of Kyiv, Kyiv, Ukraine</i>
P11	Vibration Characteristics of Double-Walled CNT@BNNT Nanotubes in Rotational Bearing Systems Merwan Behar <i>MECACOMP Laboratory, Department of Mechanical Engineering, Faculty of Technology, University of Tlemcen, Algeria</i>



Plenary lectures

Sustainable scaffolds: 3D printed bioceramic bone scaffolds for biomedical applications obtained from valorised fish wastes for the first time

Giammarco Schippa^a, Anna Bertocco^a, Marinélia Capela^b, Maria Paula Seabra^a, **Robert C. Pullar**^a

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As part of the ever-increasing importance of developing a sustainable, circular economy, as well as often for sound economic reasons, there is a growing interest in, and demand for, products produced from the valorisation of wastes and by-products of industry and agriculture. This is especially true for biomaterials, where often animal or plant wastes / by-products can offer existing natural sources for many useful products. Probably the best known bioceramic is hydroxyapatite ($\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$, HAp), the major component of human and animal bones, used for bioimplants and bone scaffolds. This can be synthetic HAp made via chemical reactions between calcium and phosphorus-containing compounds, but there is increasing development and interest in using biogenic HAp obtained from sustainable natural sources, such as animal and fish bones. These are often by-products of the food industry, which can be valorised by extracting HAp-based compounds. These naturally sourced materials exhibit biocompatibility comparable to, or superior than, that of standard commercial synthetic materials, and commercial products derived from animal bones are already available. We have previously carried out research on the conversion of wastes from the fisheries industry (fish bones and scales) into a range of HAp-based biomaterials, from fish such as cod, tuna and sardines. However, 3D printed bone scaffolds have never been produced from valorised fish wastes before. Here we report the production of 3D scaffolds made by robocasting / direct ink writing from swordfish, cod, sea bass, salmon and gilt-head bream waste bones. These are all local Italian species. The natural biogenic bioceramics produced from these are a mixture of HAp and β -tricalcium phosphate (β -TCP, $\text{Ca}_3(\text{PO}_4)_2$), which typically has an improved bioactivity and resorbability compared to pure HAp. For the first time bioceramics derived from fish wastes / residues have been 3D printed, and we report the characterisation and bioactivity of these scaffolds.

Polymer base membranes for water remediation and energy storage applications

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² *IKERBASQUE, Basque Foundation for Science, 48009 Bilbao, Spain*

³ *Physics Center of Minho and Porto Universities (CF-UM-UP) and LaPMET, Laboratory of Physics and Materials for Emerging Technologies, University of Minho, 4710-057 Braga, Portugal*

Active and multifunctional materials are being increasingly implemented in water remediation and energy storage systems. Those areas often rely on advanced membrane technology, and the development of the specific applications relies both in the ability tailor the functional response of the membrane, though the proper selection of matrix and active fillers, and on the membrane fabrication technology for obtaining a suitable membrane microstucture.

Polymer based multifunctional materials processable from solution and/or by additive manufacturing technologies is an area of increasing interest due to improved sustainability, tailorability of materials properties and simple integration into functional applications.

Relevant results, strategies and challenges in the scope of membranes for the removal of heavy metals and degradation of contaminants of emerging content will be presented, together with the approaches to improve separator membranes for battery applications. The common features of both application areas in terms of membrane development will be highlighted as well as the specificities leading to successful applications.

Carbon-Based Nanocomposites at the Crossroads of Healthcare and Environment

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Carbon-based nanocomposites have emerged as a versatile class of advanced materials with transformative potential at the interface of healthcare and environmental sustainability. Owing to their tunable physicochemical properties, high surface area, chemical stability, and functionalization versatility, these materials have attracted increasing interest for addressing critical challenges in both biomedical and environmental applications.[1] More recently, advances in artificial intelligence (AI) and machine learning are accelerating the design and optimization of these materials by predicting properties, guiding synthesis, and uncovering structure–property relationships.[2]

In the healthcare sector, carbon-based nanocomposites have shown significant promise for diagnostics, imaging, biosensing, and targeted drug delivery. In particular, CDs exhibit excellent biocompatibility, low toxicity, and outstanding photoluminescence, enabling their use as fluorescent probes for in vitro and in vivo bioimaging.[3] Furthermore, the ability to functionalize their surfaces with therapeutic agents and targeting ligands supports the development of advanced nanoplatfroms for cancer diagnosis and treatment, including chemotherapy, photodynamic therapy, and theranostic applications.

Beyond biomedicine, carbon-based nanocomposites play an increasingly important role in environmental protection and remediation.[4] Their high adsorption capacity and tunable surface chemistry make them effective materials for removing heavy metals, dyes, pharmaceuticals, and other emerging contaminants from water systems. In addition, their sensitive optical and electrochemical responses enable the development of selective sensors for environmental monitoring, facilitating the detection of pollutants at trace concentrations.

Advances in material design, functionalization, and scalable manufacturing are expected to drive the wider adoption of carbon-based nanocomposites in healthcare and environmental applications.

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Screening the hydrogen storage materials for vehicular applications

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^bLASI - Intelligent Systems Associate Laboratory, Guimarães, Portugal

Hydrogen is widely regarded as a promising energy carrier for decarbonizing the transportation sector. However, the successful deployment of hydrogen-powered vehicles requires compact, lightweight, and safe onboard hydrogen storage systems [1]. The U.S. Department of Energy (USDOE) has established a system-level gravimetric hydrogen storage target of 6.5 wt.% for light-duty vehicles. Considering that balance-of-plant (BOP) components, including storage vessels, heat exchangers, valves, sensors, and thermal management systems, typically account for approximately 30% of the total system mass, the hydrogen storage material itself must ideally deliver at least 9.3 wt.% reversible hydrogen capacity to meet the overall system target. To date, no single reversible metal hydride system simultaneously satisfies all capacity, kinetic, thermodynamic, durability, and cost requirements for vehicular applications.

This work critically screens representative reversible hydride materials that have received significant attention for onboard hydrogen storage, namely LaNi_5H_6 , NaAlH_4 , MgH_2 , and the $\text{LiBH}_4\text{--MgH}_2$ reactive hydride composite (RHC). LaNi_5H_6 exhibits excellent reversibility and rapid hydrogen sorption kinetics near ambient conditions but suffers from a very low hydrogen capacity (~ 1.4 wt.%). Sodium alanate (NaAlH_4) offers improved reversible capacity (~ 5.6 wt.%) and can be reversibly cycled with suitable catalysts; however, kinetic limitations and thermal management requirements remain significant challenges. Magnesium hydride (MgH_2) provides a high theoretical hydrogen capacity of 7.6 wt.% together with low cost, abundance, and excellent reversibility, making it one of the most attractive near-term candidates [2]. Nevertheless, its practical implementation is hindered by high desorption temperatures and sluggish hydrogen sorption kinetics. In contrast, the $\text{LiBH}_4\text{--MgH}_2$ RHC exhibits a theoretical reversible capacity of ~ 11.5 wt.%, exceeding the material-level capacity required to satisfy future USDOE targets. Despite this advantage, challenges related to reaction kinetics, thermal conductivity, cycling stability, and system integration continue to limit its practical deployment.

Based on the comparative assessment, MgH_2 appears to be a viable intermediate solution for next-generation hydrogen-powered vehicles owing to its favorable balance between capacity, cost, and technological maturity. In the longer term, reactive hydride composites, particularly $\text{LiBH}_4\text{--MgH}_2$ systems represent one of the most promising pathways toward meeting stringent gravimetric storage targets. Future research should focus on improving sorption kinetics, reducing operating temperatures, enhancing thermal management, and ensuring long-term cyclability. In this context, our research group is developing prototype MgH_2 and RHC-based metal hydride storage containers with a total system weight of approximately 2 kg, aiming to bridge the gap between material-level performance and practical vehicular hydrogen storage applications.

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Invited speakers

11. Impact of Antisite Disorder on the Resistivity of $\text{Sr}_2\text{FeMoO}_6$ Ceramics

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In this work, we consider the influence of antisite disorder (ASD), e.g., Fe ions on Mo sites, Fe_{Mo} , and vice versa, Mo_{Fe} , on the resistivity of strontium ferromolybdate ceramics fabricated by the solid-state reaction method. Strontium ferromolybdate ceramics fabricated via solid-state reactions exhibit a low-temperature minimum resistivity owing to the interplay between the bulk metallic resistivity of the grains, which increases with temperature and becomes dominant at higher temperatures, and an intergrain tunneling mechanism of charge carrier conduction, which leads to a decrease in conductivity with decreasing temperature in the low-temperature region. The parameters of the bulk metallic resistivity and fluctuation-induced intergrain tunneling were determined by fitting the experimental data to these resistivity models. The impact of antisite disorder on the resistivity parameters was considered. It turns out that antisite disorder affects the effective barrier height of intergrain tunneling and the effective values of the barrier width and the barrier area. Disorder increases the effective barrier height for intergrain tunneling, increases its barrier width, and decreases the effective barrier area of nanosized barriers. The results are discussed using experimental data available in the literature.

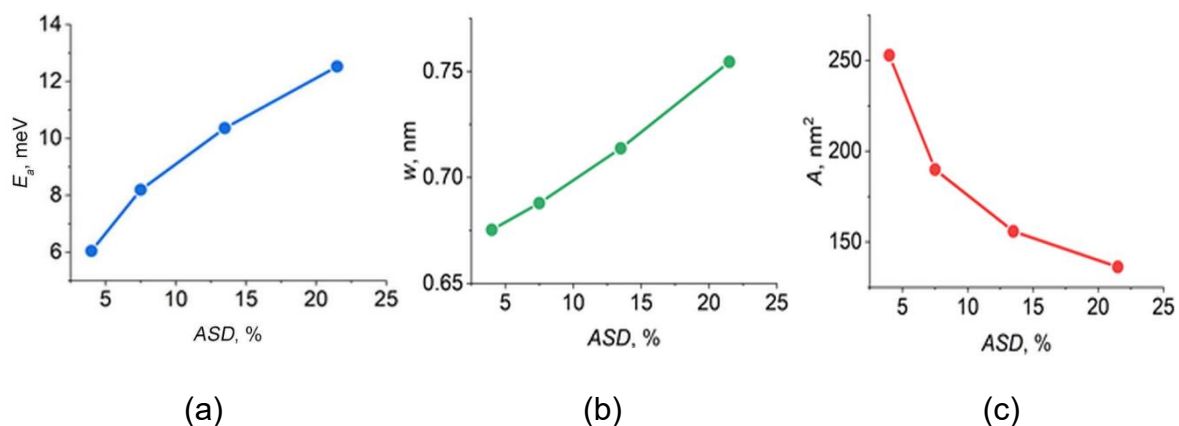


Figure 1: Effective values of the intergrain barrier height E_a (a), barrier width w (b), and barrier area A (c) depending on the value of antisite disorder (ASD).

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I2. Crystallization of amorphous $\text{Yb}_2\text{O}_2\text{S}$ films

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Amorphous $\text{Yb}_2\text{O}_2\text{S}$ films are formed on substrates at room temperature in the process of electron-beam evaporation of YbS in vacuum and subsequent oxidation at separation of the film from the substrate in distilled water. Electron beam irradiation causes their crystallization with the formation of $\text{Yb}_2\text{O}_2\text{S}$ micro crystals with hexagonal crystal lattice.

In situ electron microscopy studies with the video recording method demonstrated, that phase transformation occurs in the island polymorphous crystallization mode with the relative length $\delta_0 \approx 1030$. In this case, the dependence of the fraction of the crystalline phase x on time t has an exponential character, described by the Johnson-Mail-Avrami-Kolmogorov formula.

The formation of the film occurs at the constant crystal growth rate and at the constant intensity of nucleation of crystallization centers α , that corresponds to the α -version of the Kolmogorov's model (Fig. 1).

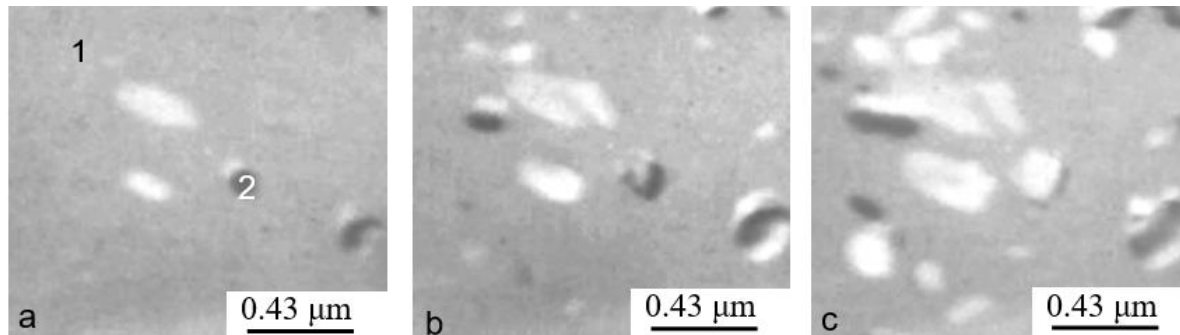


Fig. 1. Crystal growth in the amorphous film of $\text{Yb}_2\text{O}_2\text{S}$. The micrographs correspond to the periods of time t , that passed after the video recording had started: (a) $t = 1.40$ s; (b) $t = 2.03$ s; (c) $t = 2.80$ s.

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I3. Engineering Functional Cobalt Oxide Perovskites for Advanced Electronics

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Complex oxide perovskites have emerged as an important class of materials for future electronic technologies because their electronic, magnetic, and transport properties can be tailored through composition, defect chemistry, and lattice engineering. In particular, cobalt oxide perovskites exhibit a rich interplay between crystal structure, oxygen stoichiometry, charge transport, and magnetic ordering, providing opportunities for designing multifunctional materials for oxide electronics, non-volatile memories, spintronic systems, and neuromorphic computing [1-3].

This presentation highlights recent advances in engineering functional properties of cobalt oxide perovskites through crystal synthesis and epitaxial thin-film integration. Emphasis will be placed on how growth conditions, oxygen environment, and substrate-induced lattice constraints influence structural evolution and stabilize distinct electronic and magnetic states. The discussion will further demonstrate how controlled materials engineering enables the emergence of functional responses, including resistive-switching characteristics, in epitaxial oxide heterostructures.

By establishing clear relationships between synthesis, structure, and functionality, this work provides insights into the design of next-generation multifunctional oxide materials and illustrates the growing potential of cobalt oxide perovskites as a versatile platform for advanced electronic technologies.

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I4. Advanced Chalcogenide and Tellurite Glasses for Mid-Infrared Photonics, Sensing, and Light Conversion

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Functional glass materials offer remarkable opportunities for tailoring optical, structural, and spectroscopic properties through compositional engineering. In this work, research conducted in our laboratory focuses on two important classes of advanced photonic materials—chalcogenide and tellurite glasses—designed for sensing, luminescent, and photonic applications.

Chalcogenide glasses, based on sulfur, selenium, and tellurium combined with group IV–V elements, exhibit wide transparency in the mid-infrared (MIR) spectral region, high refractive indices, and low phonon energies, making them highly attractive for infrared photonics and sensing technologies. Rare-earth-doped chalcogenide glasses and optical fibers have been developed and investigated for MIR gas sensing applications. Optical absorption, photoluminescence, and lifetime measurements, together with Judd–Ofelt analysis, are employed to evaluate radiative properties and optimize luminescent performance. These materials show significant potential for the detection of environmentally and industrially relevant gases, including CO₂ and CH₄, through their characteristic MIR absorption bands.

In parallel, rare-earth (Tm³⁺ and Ho³⁺) doped tellurite glasses prepared in OH radical free environment are explored owing to their excellent glass-forming ability, high rare-earth ion solubility, broad optical transmission window, and favorable spectroscopic characteristics. Structural and optical investigations are performed to understand composition–property relationships and to optimize emission efficiency for visible and near-infrared photonic applications and temperature sensing. The combination of low phonon energy and high rare-earth incorporation enables the development of efficient luminescent materials for temperature sensing in both NIR and MIR regions besides usable for gas detection. These studies demonstrate how rational compositional design and spectroscopic optimization of chalcogenide and tellurite glasses can lead to advanced functional materials for mid-infrared sensing, luminescence, and next-generation photonic devices.

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15. Bias-voltage Induced Transition from Capacitive-coupled to Purely Resistive Switching Behaviour in Ag/PVA-Graphene oxide/FTO Devices

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Polyvinyl alcohol-graphene oxide (PVA-GO) based composite thin film devices Ag/PVA-GO/FTO were fabricated. A transition from the capacitive-coupled to purely resistive switching was observed with an increase in applied voltage and higher GO concentration. We also investigated the non-volatile, forming-free resistive switching characteristics of Ag/PVA-GO/FTO devices. The Ag/PVA-GO-0.2 wt. %/ FTO device exhibited superior bipolar resistive switching with a V_{SET} (Set Voltage) of ~ 1.72 V, a V_{RESET} (Reset Voltage) ~ 1.83 V and a switching ratio of $\sim 10^3$. This device exhibited two clearly distinct states at a read voltage of 0.1 V in both endurance and retention tests. It successfully switched for 2500 cycles and maintained its state for 4020 seconds without any noticeable degradation. Furthermore, the charge-flux linkage characteristic revealed a double-valued function, where the time domain-charge presented an asymmetric pattern, while the time domain-flux displayed a symmetric pattern. The electrical conduction mechanism and resistive switching behaviour were explained with suitable models.

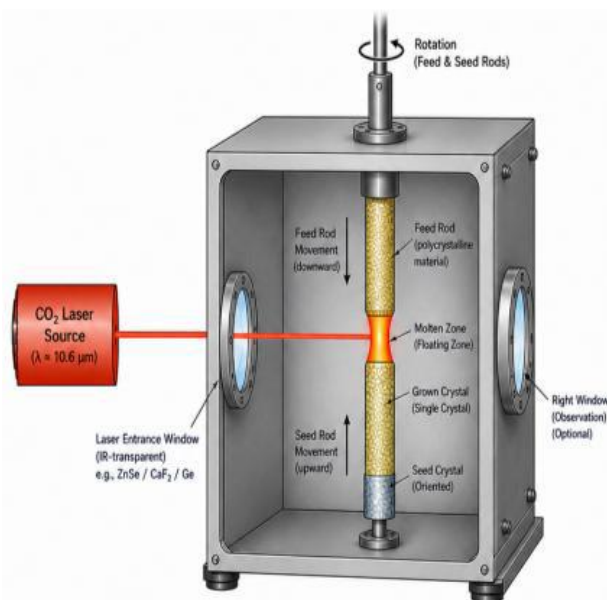
16. Spectroscopic investigations of Laser Floating Zone grown Lanthanum Aluminate crystals

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Lanthanum aluminate (LaAlO_3) is a high-temperature stable rare earth aluminate with a perovskite structure that exhibits a low dielectric constant, low microwave dielectric loss, and low phonon energy, making it an attractive substrate material for thin film growth and photonic applications. Owing to its high melting temperature ($\sim 2080^\circ\text{C}$), the growth of high-quality LaAlO_3 single crystals remains limited. The crystal structure is composed of corner-sharing AlO_6 octahedra, while the growth conditions strongly influence the formation of oxygen vacancies, antisite defects, and the resulting crystal quality. LaAlO_3 crystallizes in a pseudocubic perovskite structure above the structural phase transition temperature ($T_c \approx 813\text{ K}$) and transforms to a rhombohedral distorted structure (space group $R\bar{3}c$) at room temperature.



The Laser Floating Zone (LFZ) technique provides several advantages for the growth of refractory oxide crystals, including steep thermal gradients, rapid solidification, high growth rates, and precise control over crystal composition without the use of a crucible. In this work, LaAlO_3 crystals were grown by the LFZ method using seed and feed rods prepared from La_2O_3 and Al_2O_3 powders with polyvinyl alcohol (PVA) as a binder. Crystal growth was performed at different pulling rates using a continuous-wave CO_2 laser ($\lambda = 10.6\text{ }\mu\text{m}$) operated at a fixed power of approximately 75 W. Phase identification by powder X-ray diffraction (PXRD) combined with Rietveld refinement confirmed the formation of single-phase rhombohedral LaAlO_3 with space group $R\bar{3}c$. Raman spectroscopy further verified the rhombohedral phase through the characteristic low-frequency phonon modes associated with the distorted AlO_6 octahedral framework, while Fourier transform infrared (FTIR) spectroscopy revealed the characteristic La–O and Al–O vibrational modes. The influence of pulling rate on crystal growth behaviour, microstructure, and the evolution from polycrystalline to single-crystal growth was systematically investigated. These results demonstrate that the LFZ technique is an effective approach for the growth of high-quality LaAlO_3 single crystals and provides a structural basis for the future incorporation of rare-earth activator ions for advanced optical and photonic applications.

17. Cubic Niobium Oxynitride: A Novel Electrode Material for Proton Ceramic Membrane Reactors

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Proton ceramic membrane reactors (PCMRs) are increasingly recognized for their ability to operate on ammonia-based fuels to generate electricity and, conversely, to synthesize ammonia from electricity and steam or hydrocarbons at ambient pressure^{1,2,3}. This approach offers significant advantages over the conventional Haber–Bosch process, including lower costs and reduced carbon emissions^{1,4}. However, the development of suitable electrode materials remains a major challenge. In this study, niobium (oxy)nitride (NbN_xO_y) was investigated as a potential electrode component in a composite with a proton-conducting perovskite ceramic⁵.

The processed materials were characterized using a range of techniques, including X-ray diffraction (XRD), thermogravimetric and differential scanning calorimetry (TGA/DSC), scanning electron microscopy coupled with energy-dispersive spectroscopy (SEM/EDS), dilatometry, and impedance spectroscopy (IS). The results demonstrated the chemical compatibility of NbN_xO_y with a proton-conducting ceramic electrolyte and enabled the development of a fabrication route for composite electrodes. Furthermore, a mechanistic investigation of electrode behavior under reducing atmospheres was carried out using a symmetrical cell configuration.

BCZY712 exhibited chemical stability up to 850 °C, facilitating the sintering of the electrode films. Thermogravimetric analysis and X-ray diffraction revealed that NbN_xO_y decomposes into its parent oxides in N_2 , while maintaining phase purity under reducing conditions. The polarization behavior of the BCZY712– NbN_xO_y composite electrode was evaluated by impedance spectroscopy under different atmospheric conditions. The observed electrochemical response suggests a reaction mechanism involving proton incorporation and water management, hydrogen adsorption/desorption processes, and interfacial charge-transfer reactions associated with protons and/or oxygen-vacancy defects.

Overall, this work presents a systematic approach to the processing, fabrication, chemical stability assessment, and electrochemical characterization of a novel composite electrode comprising niobium (oxy)nitride (NbN_xO_y) and a proton-conducting perovskite ceramic, highlighting its potential for application in proton ceramic membrane reactors.

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18. Yttrium-doped barium stannate: A carbonation-resistant perovskite anode component for proton ceramic electrochemical cells

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Proton ceramic electrochemical cells (PCECs) demand anode electrode materials that withstand a strongly reducing, humid, and carbonaceous fuel-electrode environment. State-of-the-art barium cerates offer high proton conductivity but carbonate in CO₂/H₂O, while barium zirconates are stable yet refractory [1]. Here we evaluate yttrium-doped barium stannate, BaSn_{0.8}Y_{0.2}O_{3-δ} (BSY), in which the more acidic Sn⁴⁺ B-site confers intrinsic carbonation resistance [2]. Phase-pure cubic BSY (*Pm-3m*, *a* = *b* = *c* = 4.1806 Å) was synthesised mechanochemically and shown by powder X-ray diffraction to remain single-phase across dry and humidified H₂, CH₄, and CO₂ at 800 °C. Decomposition occurs only above 900 °C in H₂ and is driven by B-site redox (Sn⁴⁺ → Sn²⁺ reduction, confirmed by X-ray photoelectron spectroscopy). Ni-BSY||BSY||Ni-BSY symmetrical cells were co-fired between 1000 °C and 1400 °C, with 1300 °C giving optimal porosity, intimate Ni-BSY mixing, and the lowest ohmic resistance; at 1400 °C nickel dissolves into the lattice, depleting the effective acceptor content and raising ohmic resistance. Impedance spectroscopy under wet H₂ reveals an ohmic contribution with a temperature dependence reflecting a transition from proton-dominated transport (*E*_a = 0.34 – 0.56 eV) at low temperature to oxygen-ionic and emerging n-type conduction at high temperature, together with a single electrode arc whose apparent polarisation resistance requires correction for electronic leakage. These results establish BSY as a chemically robust anode component for intermediate-temperature PCECs.

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19. Piezoelectric polycrystalline thin films of dileucine for energy harvesting

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Piezoelectric energy harvesting devices can power small implantable medical devices, such as biosensors or drug delivery systems, without the need for traditional batteries harmful for the human body. Organic piezoelectric thin films made of dipeptides are flexible and naturally biocompatible [1]. Though the choice of amino acids in the peptide sequence is crucial for the peptide assembly, the diphenylalanine (H-Phe-Phe-OH, FF) dominates in the reports in until now. Here we demonstrate the ability of dileucine (H-Leu-Leu-OH, LL) to form well-ordered polycrystalline films with strong piezoelectric properties attractive for biomedical applications. We used a spin coating technique to form homogeneous amorphous films with the thickness below 300 nm and implemented their crystallization by water or isopropanol vapor exposure. Water-treated films consist of ordered LL nanotubes, whereas isopropanol-treated films represent another polymorphic form of LL rarely reported in literature [2]. Quantum-chemical calculations allowed to estimate the films' polarization, whereas piezoelectric force microscopy has revealed pronounced lateral piezoelectric response with a shear piezoelectric coefficient $d_{15} = 8.9\text{--}12.8$ pm/V that is comparable with ZnO and CdS (8.3 and 13.9 pm/V, respectively [3]). Further optimization of the film's preparation can improve the response and make it comparable with that observed in FF films (80 pm/V [1]).

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I10. Synthesis of Highly Crystalline Microdiamonds via Nano-Silicon Assisted Liquid Metal CVD

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We report an ambient-pressure liquid-metal-assisted CVD strategy that enables shape-programmable growth of micro-scale diamond by coupling a-liquid-metal Ga–In alloy with ferrocene ($\text{Fe}(\text{C}_5\text{H}_5)_2$) as a carbon precursor, nanodiamond seeds, and nanosilicon. Building on liquid-metal diamond synthesis,^{1,2} this approach enables pushes liquid-metal growth toward a low temperature (900 °C, 1 atm) while enabling single-crystal diamonds to be scaled from $\sim 10\text{ }\mu\text{m}$ to several tens of micrometers with well-developed faceting.³ Ferrocene decomposition supplies a sustained interfacial carbon flux that is captured and redistributed by the Ga–In melt toward seed-rich liquid–solid interfaces. Defect-rich nanodiamond provides the crystallographic template required for reliable sp^3 nucleation despite the intrinsically low carbon solubility of Ga–In. Nanosilicon plays a distinct, complementary role by tuning interfacial kinetics and facet competition, enabling deliberate control of crystal habit: cubic ($\sim 10\text{ }\mu\text{m}$), truncated-tetrahedral, and fully faceted octahedral diamonds are reproducibly obtained by adjusting the nanosilicon: nanodiamond ratio,⁴ with octahedral crystals reaching $\sim 50\text{ }\mu\text{m}$. Importantly, crystal size is further scaled by regulating hydrogen flow: lowering the H_2 rate increases net carbon retention at the liquid-metal interface, raises effective supersaturation, and accelerates diamond deposition. Together, habit control (via nanosilicon: nanodiamond) and size scaling (via H_2 flow) establish a practical route silicon-drive facet regulation and size under ambient pressure, offering a pathway to tunable micro-sized single-crystal diamonds under mild conditions

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Oral presentations

O1. Tensile Mechanical Properties of Goldene Nanotubes: A molecular Dynamics Simulation

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A recent breakthrough in two-dimensional nanomaterials reported the first synthesis of goldene (a single-atom-thick gold lattice) via wet-chemical removal of Ti_3C_2 from layered Ti_3AuC_2 [1]. As the first stable monolayer metal sheet, goldene is expected to exhibit novel physics reminiscent of graphene [2]. Rolling up goldene produces gold nanotubes (GNTs), which, with tunable sizes and shapes, hold promise for diverse applications such as filtration and electrical interconnects. This study aims to investigate the mechanical properties of gold nanotubes using molecular dynamics (MD) simulations. All simulations were performed with the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package [3]. The Nosé–Hoover thermostat was applied for temperature control, and periodic boundary conditions (PBC) were employed to manage the number of atoms. Stress–strain diagrams were obtained from MD tensile tests. Furthermore, the effects of temperature, nanotube radius, edge orientation, length, vacancy defects, and stretching rate on the mechanical properties of GNTs were systematically examined. These findings provide critical insights for the design and application of gold nanotube-based nanodevices.

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O2. Sustainable production of Fe-Ni alloy from nickel iron oxide by electroreduction in strongly alkaline suspensions

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The potential of extending renewable-energy-powered electrochemical routes towards green steelmaking through the direct production of Fe-based alloys was investigated. A mixed spinel-type oxide (NiFe_2O_4) was used as a precursor for the electrodeposition of Fe-Ni alloys in a strongly alkaline solution. The electrochemical activity of the precursor oxide, the possible reduction pathways, and the structural and compositional characteristics of the deposits produced were evaluated. Compared with simple oxide mixtures ($\text{Fe}_2\text{O}_3 + \text{NiO}$), NiFe_2O_4 containing electrolytes revealed higher concentrations of dissolved Ni, as determined by ICP-MS, suggesting that the spinel structure favours Ni availability in strong alkaline solutions. XRD patterns confirmed the formation of a Fe-Ni phase in deposits derived from the single oxide precursor. In contrast, deposits formed from oxide mixtures represent metallic Fe and residual NiO, suggesting incomplete reduction. Structural and microstructural characterization by EELS, supported by HRTEM, SAED, EDX, and XRD analyses, revealed compositional heterogeneity of the deposits, but confirms successful alloy formation. The combined results support a possible hybrid interfacial mechanism, involving particle adsorption at the cathode, local solid-state reduction of activated NiFe_2O_4 particles, surface hydroxylation/reconstruction and limited dissolution of electroactive species. The Faradaic efficiency increased ~30% when the NaOH concentration was raised from 10 M to 18 M, indicating the role of electrolyte alkalinity towards Fe-Ni alloy electrodeposition. Overall, the results demonstrate that mixed oxides, such as spinel-type NiFe_2O_4 provide a promising platform for alloy electrodeposition in alkaline suspensions and can outperform mixtures of individual oxides.

O3. Catalyst and support engineering for next-generation passive autocatalytic recombiners

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The safe management of hydrogen (H₂) under accidental release conditions remains a critical requirement for nuclear, industrial, and emerging H₂ energy systems. Passive Autocatalytic Recombiners (PARs) offer an inherently safe and maintenance-free approach to mitigate H₂ build-up and formation of explosive mixtures with air through catalytic H₂/O₂ recombination. This work presents recent advances at North-West University, HySA Infrastructure in catalyst and support engineering aimed at enhancing PAR performance, stability, and resilience under diverse operating conditions.

Development efforts focused on three integrated material strategies: (1) support modification [1, 2], (2) bimetallic catalyst development [3, 4], and (3) catalyst geometries [2, 5, 6]. Support modification included Zn doping and mixed oxide formulations incorporating Zr, Ce, and Y to alter thermal stability and metal–support interactions. These doped oxides demonstrated improved dispersion of noble metals and enhanced resistance to thermal degradation. Parallel efforts on bimetallic catalysts, specifically Pt–Pd and Pt–Co systems, enabled optimization of both low-temperature and low-reactant activation. Synergistic effects between metals led to improved H₂/O₂ recombination initiation thresholds, higher recombination rates, and reduced noble-metal loading requirements.

To complement material innovations, structured catalyst geometries have been considered, including coated plates, spherical substrates, and metallic foams, to improve gas–solid contact, heat management, and scalability for industrial recombiners.

Overall, the integration of doped supports, bimetallic catalysts, and different catalyst geometries demonstrates a promising pathway toward next-generation PAR technologies with enhanced performance, robustness, and cost efficiency. These developments contribute to safer H₂ deployment across energy, industrial, and nuclear sectors, supporting the broader transition to a H₂ economy.

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O5. In-Situ Hydrothermal Design of Metal Chalcogenides Decorated 2D Materials Nanocomposites as Artificial Peroxidase Enzyme

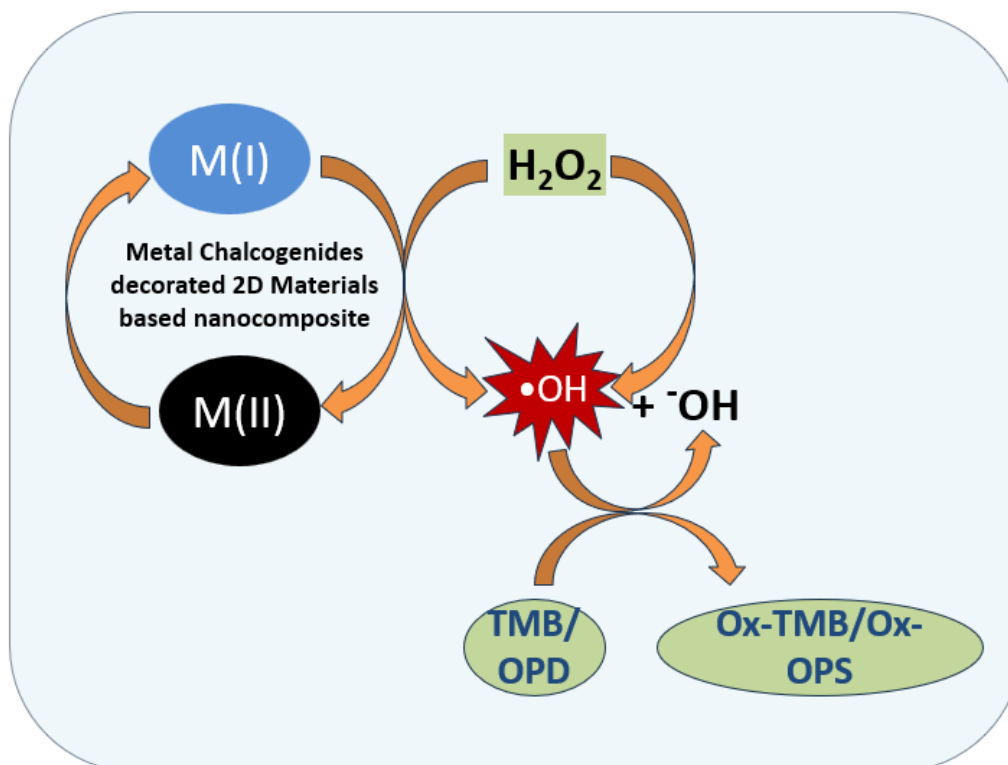
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Metal Chalcogenides Decorated 2D-nanocomposites (MXene/rGO), belonging to the family of metal chalcogenides and 2D materials, were synthesized via a facile hydrothermal method employing appropriate chalcogen source, metal salt as precursors. The material was characterized systematically using various analytical techniques, including powder X-ray diffraction (PXRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and energy-dispersive X-ray spectroscopy (EDX). Characterization techniques confirmed that the formation of nanocomposite and it possess a hexagonal morphology. This study employs a series of carefully designed experiments to validate the intrinsic peroxidase-like activity of nanocomposite, as well as to evaluate their effectiveness across a range of related structures. Nanocomposite can convert peroxidase substrates (TMB and OPD) to colored products in the presence of H₂O₂. In addition, the as-prepared nanoparticles have the potential to oxidize DPPH and ABTS substrates. Michaelis-Menten constant K_M value for TMB and H₂O₂ was found to be 12 mM and 0.60 mM for H₂O₂ and the V_{max} value of the FeSe₂ was found to be TMB and H₂O₂ was 2.50 x 10⁻⁷ and 0.82 x 10⁻⁸ MS⁻¹. These data are found to be almost comparable with natural peroxidase HRP and other artificial enzymes reported in the literature. The natural peroxidase-like activities of nanocomposite originated from the catalytic decomposition of H₂O₂ into •OH radical.



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O6. Smart Hybrid Nanozymes for Portable and Reagentless Colorimetric Sensing and Point of Care Detection

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The increasing demand for rapid, reliable, and environmentally friendly analytical platforms has driven the advancement of nanostructured materials that mimic natural enzymes for colorimetric and optical biosensing. This work unifies a series of novel research developments focused on designing multifunctional hybrid nanocomposites with enhanced catalytic and sensing capabilities for non-enzymatic detection of biologically and environmentally significant analytes. Beginning with the fabrication of Cr₂O₃–TiO₂ nanocomposite–modified filter paper sensors, a simple, portable, and highly sensitive platform was demonstrated for hydrogen peroxide (H₂O₂) detection. The synergistic coupling of Cr₂O₃ and TiO₂ endowed the system with remarkable peroxidase-like activity, enabling a low detection limit (0.003 μM) and rapid, visible color transition from green to blue within seconds—offering a prototype for point-of-care and environmental monitoring devices. Building upon this foundation, zirconium-decorated graphene oxide (Zr–GO) composites were introduced as an eco-friendly nanozyme with intrinsic catalytic activity. The Zr–GO hybrid leveraged zirconium’s green catalytic properties and GO’s exceptional surface area to achieve fast electron transfer, decomposing H₂O₂ into hydroxyl radicals for the optical oxidation of chromogenic substrates within two minutes. This recyclable and reagent-efficient system presented high sensitivity (LOD: 0.57 μM), operational simplicity, and potential for sustainable analytical chemistry.

Expanding the application domain toward biomedical diagnostics, a DMAP-functionalized MoS₂–GO hybrid was engineered for reagentless, chromogenic substrate-free visual detection of dopamine (DA)—a critical neurotransmitter linked to neurological disorders such as Parkinson’s and Alzheimer’s diseases. The hybrid’s synergistic MoS₂–GO structure offered abundant active sites and excellent redox performance, while DMAP surface functionalization enabled selective DA recognition through specific surface complexation and oxidation mechanisms. The developed system exhibited an ultra-low detection limit (0.17 μM), outstanding selectivity against interfering biomolecules, and high reproducibility in human serum analysis. Furthermore, the translation of this chemistry into paper-based test strips provided a rapid, low-cost visual assay for real-time detection in under three minutes.

Collectively, these studies demonstrate a coherent research strategy advancing from inorganic nanozymes to hybridized and surface-engineered smart biosensing materials. The integration of transition metal oxides, chalcogenides, and graphene derivatives yields multifunctional, stable, and portable colorimetric systems that bridge laboratory analytics with point-of-care diagnostics. This versatile framework paves the way for next-generation nanozyme platforms capable of reagentless, eco-friendly, and real-sample-compatible detection of diverse biomedical and environmental targets.

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O7. Electrochemical evaluation of Ni-based composite electrodes for alkaline hydrogen evolution

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Alkaline water electrolysis (AWE) is a mature technology for green hydrogen production aligned with the energy transition towards decarbonization [1]. AWE typically relies on Ni, stainless steel, Ni-based alloys and other electrode materials. MAX phases [2], a family of carbide and nitride materials, have attracted increasing attention mainly as precursors of MXenes [3], which are widely investigated for electrochemical and energy-related applications. In contrast, the direct incorporation of MAX phases into electrode architectures for alkaline hydrogen evolution remains comparatively underexplored. This work explores the processing of Ni containing MAX phase-based composite electrodes as electrocatalysts for the hydrogen evolution reaction under strong alkaline media.

Several electrode architectures were explored: i) Ti₃AlC₂ MAX phase (10 wt%) co-pressed with Ni and ii) Ti₃AlC₂ MAX phase (30 wt%) in a porous Ni–Al matrix. Alkaline water electrolysis tests were performed in a PTFE cell with NaOH electrolyte (10 M) at 25-50 °C, with a Pt wire as a counter electrode and a reference electrode of Hg|HgO|NaOH (1 M). A VERTEX.S (IVIUM technologies) potentiostat/galvanostat was used for chronoamperometry (CA) and cyclic-voltammetry studies (CV). Combined XRD/SEM/EDS studies were used to assess phase composition and microstructural characterisation of the electrodes before and after the alkaline electrolysis tests. After 4 days of CA tests (– 1.3 V vs. Hg|HgO), both electrodes showed progressive surface restructuring, including partial Al removal, increased porosity and surface roughness. These transformations resulted in clear self-activation behaviour, reflected by enhanced hydrogen evolution reaction (HER) activity and a significant increase in the electrochemically surface area (ECSA). MAX phase/Ni–Al composite electrodes demonstrated superior mechanical integrity and electrochemical performance.

Ni–Al composite electrodes constitute a promising approach for alkaline hydrogen production, in which electrochemically surface evolution and self-activation can be achieved.

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O8. Engineering Nested NiPd Nanostructures by Reactive Laser Ablation for Advanced Selective Hydrogenation Catalysis

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Catalysts are central to efficient and selective reduction processes that underpin the fine chemical, pharmaceutical, and energy industries [1]. A persistent challenge in this field is the development of catalytic systems that simultaneously exhibit high activity, selectivity, and long-term stability while being produced through sustainable and environmentally benign synthesis routes. In this contribution, we report a novel class of nested NiPd nanoparticles (NPs) synthesized via Reactive Laser Ablation in Liquids (RLAL), a green, surfactant-free technique that enables precise control over composition, phase distribution, and nanostructure formation [2].

Structural and physicochemical characterization reveals a unique nested architecture composed of alloyed NiPd domains with finely tuned electronic and magnetic interactions. This architecture translates into exceptional catalytic performance in selective hydrogenation reactions. In the benchmark reduction of 4-nitrophenol, the NiPd NPs achieve a high turnover frequency of 3680 h⁻¹ with 98.5% selectivity. Furthermore, the catalysts demonstrate outstanding chemoselectivity in the hydrogenation of nitroarenes to anilines, reactions of significant relevance to the production of dyes, agrochemicals, and pharmaceutical intermediates. The nanoscale synergy between Ni and Pd enhances both catalytic activity and operational stability, clearly outperforming monometallic counterparts and physical metal mixtures [3].

Beyond catalytic efficiency, the nanostructures exhibit tunable magnetic properties (14.4 - 27.5 emu·g⁻¹), offering promising opportunities for catalyst recovery and recyclability, an important consideration in heterogeneous catalysis and process engineering. By exploiting the non-equilibrium conditions inherent to RLAL, this contribution achieves a level of structural and compositional control that is difficult to attain using conventional wet-chemical approaches. These findings highlight RLAL as a powerful platform for the rational design of multifunctional nanomaterials with integrated catalytic and magnetic functionalities, paving the way for future progress in next generation precise nanocatalyst design.

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O9 Mechanistic Insights into the Structural, Electrochemical, and Charge-Storage Behavior of CNT@NiO Electrodes for High Capacitance and Durable Supercapacitors

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Although Li-batteries remain widely in use, there is a new shift to alternative energy storage solutions, such as supercapacitors (SCs), which offer high power output, a lasting lifespan, rapid charge-discharge capabilities, low cost, and eco-friendliness. Herein, spray pyrolysis, a facile and cost-effective method, was employed to deposit pure nickel oxide (NiO) and a composite with carbon nanotubes (CNT@NiO) at 350 °C for use as supercapacitor electrodes. The structures and morphologies of the materials were probed. Scanning electron microscopy (SEM) analysis revealed that pristine NiO nanoparticles had an irregular shape, whereas the composite exhibited a cylindrical morphology. According to Brunauer-Emmett-Teller (BET) analysis, the specific surface area of the composite was measured at 46.51 m² g⁻¹, which is greater than the 29.55 m² g⁻¹ observed for pristine NiO, and the average pore diameter was 27.37 nm, surpassing NiO's 6.10 nm. Their electrode performances were assessed through standard electrochemical tests. The findings revealed that incorporating CNTs considerably elevated the composite material's electrochemical characteristics. When tested in 2M KOH within 0-0.7 V potential, the CNT@NiO electrode supplied an exceptional specific capacitance (C) of 472.4 F g⁻¹ at 2 A g⁻¹, far greater than pristine NiO's 18.92 F g⁻¹. Additionally, the composite exhibits a 68.8% rate capability (13.6% for NiO) and 93.3% cyclic stability (81.5% for NiO) at 2 A g⁻¹ after 1,000 cycles, indicating its suitability for high-performance supercapacitors (SCs). These favorable results point to two deductions: (i) CNT@NiO is an outstanding candidate for energy storage, and (ii) spray pyrolysis is an affordable and effective electrode material fabrication method. Two novelties regarding the use of spray pyrolysis as a fabrication technique are presented in this work: (i) an in-depth discussion on reasons for prolonged cycle life in connection with structural modifications, and (ii) investigation and comparison of the Faradaic and capacitive charge storage contributions of the synthesized materials. Overall, this study presents a viable path toward locally fabricated, efficient energy storage systems that can drive the adoption of clean energy in Africa and help bridge the global energy gap.

O10. Growth, interfacial reactions, and properties of diamond and BDD thin films grown by MPCVD on Nb-coated silicon

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Diamond and boron-doped diamond (BDD) thin films have great technological significance, owing to their exceptional characteristics including but not limited to hardness, chemical inertness, high thermal conductivity, and tunable electronic properties. Advancement in their manufacturing technology, particularly Microwave Plasma Chemical Vapour Deposition (MPCVD), has enabled the fabrication of high-quality diamond coatings on a wide range of substrates. Here in this study we present the diamond and BDD film growth on a silicon (Si) substrate coated with niobium (Nb) layer, which was aimed to be used as metallic interlayer for controlling adhesion of diamond film. Additionally, owing to our experience of the system, in-situ formation of intermetallic compounds like niobium silicide (NbSi₂) have to be formed and employed for diamond coating characteristics.

Diamond films were synthesized on silicon and Nb-coated silicon substrates, and their structural, morphological, and chemical properties were systematically investigated. Diffraction, spectroscopic and microscopic analyses confirmed formation of the desired diamond coatings on the anticipated interlayer. Depending on the fabrication conditions, precursor compositions, and substrate types, different films have successfully been achieved. The films were employed in electrochemical systems to study their energy storage performance as supercapacitors and also investigate their catalytic role in hydrogen evolution reaction (HER) and oxygen evolution reaction (OER).

O11. Micronutrient-loaded Chitosan-Polyethylene Glycol Nanocomposite Coatings: Synthesis, Characterization, and Field Evaluation for Improved Wheat Germination and Productivity

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This study focuses on developing chitosan-polyethylene glycol (Cs-PEG) nanocomposite coatings incorporated with zinc oxide nanoparticles (ZnO NPs) for agricultural applications. The Cs-PEG film exhibited a semi-crystalline structure with enhanced water retention and a granular porous surface, making it ideal for seed coating and soil conditioning. The addition of ZnO NPs improved the film's hydrophilicity and structural integrity. Characterization techniques confirmed the hexagonal wurtzite crystalline structure of ZnO NPs and their interaction with the Cs-PEG matrix. Field trials showed that Cs-PEG-ZnO coatings significantly enhanced wheat germination (up to 100%), growth parameters (shoot length, root length, tillers per plant, spike length, grain yield), and zinc uptake. The coating demonstrated controlled zinc delivery, reduced leaching, and improved agronomic performance. The study highlights the potential of Cs-PEG-ZnO coatings as a sustainable strategy for seed biofortification, improving crop productivity while ensuring micronutrient management. The optimal balance of hydrophilicity, structural integrity, and biodegradability makes Cs-PEG-ZnO a promising superabsorbent material for agricultural applications, with potential benefits for crop growth and yield.

O12. Peptide functionalized phase convertible targeted nanodroplets for ultrasound triggered drug release across Blood Brain Barrier

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Ultrasound (US), as a non-invasive and non-ionising technology, has been utilized as an efficient technique for transporting drugs and genes across physiological barriers, such as the blood-brain barrier (BBB), in addition to its use in medical imaging. In Contrast-Enhanced Ultrasound Imaging (CEUS), microbubbles act as an effective delivery vehicle, thereby enhancing cellular uptake of the drug. This characteristic is attributed to the cavitation property of the microbubbles. In this study, we synthesised gH625-tagged pre-Polyglycerolsebacate encapsulating a perfluoropentane core (Pre-PGS-PFP) nanodroplets with improved internalisation properties and the ability to deliver a payload by phase converting to phase convertible nanodroplets upon insonation. Amygdalin, as an anticancerous drug, was loaded in the polymeric shell of Pre-PGS-PFP phase convertible nanodroplets using the solvent displacement method and was conjugated to the membrane-crossing peptide (gH625) using NHS-EDC coupling. The nanodroplets were physicochemically characterized using FTIR, SEM, confocal microscopy and zeta analysis. The nanodroplets were found to load 80.10% of Amygdalin. Cytotoxicity and uptake studies in U87 glioblastoma cells demonstrated that ultrasound-triggered amygdalin release significantly enhanced cell death compared to diffusion-based release or treatment with free Amygdalin. Furthermore, the presence of gH625 further improved cellular uptake due to its membrane-penetrating ability. Overall, the synergistic effect of ultrasound activation and gH625 functionalization facilitated efficient internalization and localized drug release, suggesting a promising strategy for targeted delivery and therapeutic enhancement in the treatment of glioblastoma.

O13. High performance of Ag/AlN/Si Schottky diode: Study of the DC sputtering power effect on its electrical properties

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The DC sputtering power (DCSP) effect on the chemical composition, structural and electrical properties of Ag/ AlN/Si Schottky diode was studied. The AlN films grown on Si substrate were examined by X-ray diffraction (XRD), Fourier Transformed Infra-Red (FTIR), and Raman spectroscopy. The analyzes by XRD, FTIR and Raman show stability at the level of the structure and the qualitative chemical composition of the AlN layer for DCSP of 200 W and 400 W. However, the quantity of chemical compounds on the surface of AlN is affected by this variation. From Current-Voltage (I-V) measurements, the ideality factor (n), barrier height (ϕ_b), and series resistance (R_s) were extracted by adopting Cheung functions. Diodes with an AlN interlayer elaborated at 400 W have good rectifying behavior with n , R_s and ϕ_b of 3.11, 1930 Ω , and 0.93 eV, respectively. The enhancement of the Ag/AlN/Si diode performance was attributed to the reduction of undesirable impurities in the Ag/AlN interface as well as the morphological improvement of the AlN layer. Capacitance-Voltage (C-V) measurements showed that carrier donor concentrations are strongly affected by DC sputtering power. The elaborate structures may provide new materials with electrical properties having a wide range of applications in electronics and photovoltaic field.

O14. Structure–Tribology Correlations of Imidazolium- and Phosphonium-Based Green Dispersants for Carbon Stabilization in Oil

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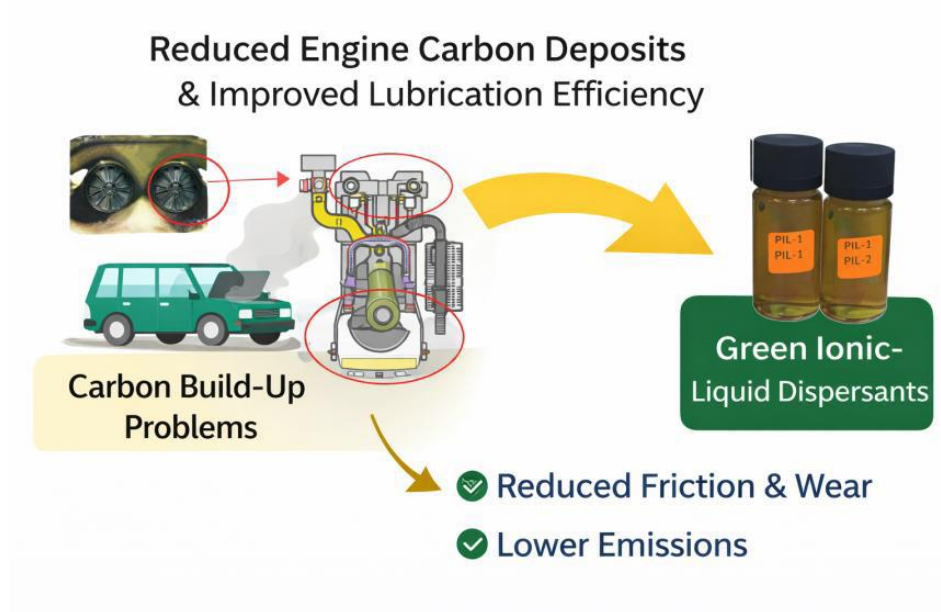
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Stabilizing carbonaceous particles in low-dielectric engine oils is essential for developing energy-efficient lubrication systems that mitigate frictional losses, greenhouse gas emissions, and airborne particulate formation. In nonpolar lubricants, the large Bjerrum length suppresses particle charging, rendering electrostatic stabilization ineffective and promoting aggregation, which limits the performance of conventional dispersants [1,2]. In this work, imidazolium- and phosphonium-based polyisobutylene ionic liquids (PILs) are investigated as green dispersants designed to address these challenges through combined electrostatic and non-electrostatic mechanisms. Surface-tension measurements confirmed early-stage micelle formation at low PIL concentrations, indicating spontaneous interfacial self-assembly. UV–Vis spectroscopy quantified PIL adsorption on carbon surfaces, with Langmuir and Freundlich analyses revealing high adsorption capacity and strong surface affinity, consistent with both monolayer and heterogeneous adsorption behavior depending on dispersant concentration. Multiscale structural characterization using small-angle neutron scattering (SANS-2D) and small-angle X-ray scattering (SAX) resolved nanoscale dispersant organization and particle–dispersant interactions. Model analysis revealed a concentration-dependent stabilization mechanism, transitioning from long-range electrostatic effects at low PIL loadings to steric-dominated stabilization at higher concentrations driven by excluded-volume effects of bulky alkyl substituents. At excessively high concentrations, carbon reaggregation was observed and attributed to depletion interactions, which are well described by Asakura–Oosawa theory linking polymer-induced osmotic pressure to effective particle attraction. Four-ball wear testing under boundary-lubrication conditions demonstrated significant reductions in friction and wear, linking nanoscale dispersant structuring and adsorption behavior to macroscopic lubrication performance and energy efficiency. This study establishes a comprehensive nanostructure–adsorption–tribology framework for PIL-based dispersants in low-dielectric oils, highlighting their potential as sustainable additives for engine lubrication systems aimed at reducing wear, improving efficiency, and lowering particulate emissions.



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O15. What role does artificial intelligence play in modern mechanical and material engineering?

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Artificial Intelligence (AI) plays a critical role in the evolution of mechanical and material engineering by enabling data driven analysis, intelligent automation, and enhanced system performance. Through the use of advanced algorithms, AI can process large amounts of data generated from simulations, experimental testing, and sensor based monitoring systems to support accurate prediction and optimization. In modern mechanical and material engineering, AI is widely applied in areas such as predictive maintenance, fault diagnosis, design optimization, intelligent control systems, vibration analysis, and advanced manufacturing processes. The integration of AI techniques improves efficiency, reduces downtime and operational costs, and enhances the reliability of mechanical systems. As mechanical systems continue to grow in complexity, AI has become an essential tool for developing smart, adaptive, and high performance engineering solutions. This study aims to review recent advancements in the application of AI across several key area of mechanical engineering, including predictive maintenance and condition monitoring, intelligent design and optimization of mechanical components, robotics and autonomous systems, smart manufacturing and Industry, thermal and fluid system analysis, and vibration and structural health monitoring, materials discovery and design, microstructure analysis, and prediction of material properties and degradation behavior. By examining these development, the study highlights how AI driven approaches are reshaping traditional mechanical engineering applications and enabling more efficient, adaptive, and intelligent engineering solutions.

O16. Preparation of bioplastic films from *Abelmoschus esculentus* by Microwave Assisted Extraction: Influence of microwaving time on the film's properties

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Comprehensive investigations of polysaccharides are essential for the fundamental understanding of their properties in exploiting them due to their potential as bio-composites and nano-conjugates in the packaging sector. Polysaccharides are considered to be superior to other polymers due to their ease in tailoring, bio-compatibility, bio-activity, homogeneity and bio-adhesive properties. In this study the extraction of okra pod mucilage (OPM) using microwave assisted extraction (MAE) at 320W with different extraction times (1-4 min) and hot water-assisted extraction (HWE) was done. Thereafter, OPMs were dried at $(28 \pm 1)^\circ\text{C}$ to obtain okra pod mucilage films (OPMF), which were characterised by infrared spectroscopy (FTIR), evaluation of the degree of esterification (DE), solubility and pH in some polar solvents (distilled water (H₂O); Ethanol (EtOH) and Dimethylsulfoxide (DMSO)). On the organoleptic properties, the OPMFs exhibited a pleasant smell characteristic of sugars. The FTIR spectra confirm the presence of bands characteristic of OPM polysaccharides and the values of DE (6.46 – 9.87%) suggest an influence of the microwave treatment time on the esterification rate. The obtained OPMFs had contrasting solubility (52-86% in H₂O, 4-46% in EtOH, 0-58% in DMSO) and pH (4.62-7.42 in H₂O, 6.07-6.86 in EtOH, 6.07-6.69 in DMSO) owing to the influence of MAE time on the structural characteristics of OPMF. This study shows that a variation in MAE time influences the structural and physicochemical properties of OPMF. This can be used to prepare OPMF with tailored properties for specific applications in different industrial sectors. In line with the exhibited properties of OPMF, applications in drug delivery systems are suggested.

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O17. Spiropyran-coated magnetite used for pollutant removal

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The demand for water treatment is anticipated to rise due to the European Environmental Regulations for Water Quality, which aim to lower contaminant concentration limits in drinking and surface water by 2036, thereby increasing the need for advanced and intelligent materials in wastewater management [1]. The development of intelligent and stimuli-responsive materials represents a potential alternative in advanced water treatment technologies, going beyond catalytic efficiency.

In recent years, in wastewater treatment technologies, increasing attention has been given to advanced oxidation processes (AOPs) because they are effective at removing several emerging contaminants. The processes, primarily comprising electrochemical oxidation, ozonation, photo-Fenton-like methods, and UV/H₂O₂ techniques, demonstrate a significant ability to produce reactive oxygen species (ROS) under ultraviolet light, including hydroxyl ($\bullet$ OH) and hydroperoxyl (HO₂ $\bullet$) radicals, which are strong and non-selective chemical oxidants that efficiently degrade a variety of organic compounds at high reaction rates [2-4].

Bisphenol A (BPA) is a widespread microplastic pollutant that presents significant environmental concerns by activating estrogen receptors and inducing hormonal disorders, posing serious risks to human health [5-7]. Inspired by natural systems, similar dual-molecule or synergistic systems are designed and synthesized in the laboratory for a comprehensive examination of the efficient degradation of pollutants, particularly BPA. Electron Spin Resonance (ESR) spectroscopy experiments show that spiropyran-coated magnetite nanoparticles can efficiently produce ¹O₂ (about 59 μ M of ¹O₂ in only 60 minutes) in aqueous suspension while maintaining stable operational conditions. The catalytic activity of the obtained nanoparticles exhibited pseudo-first-order kinetics in all photodegradation reactions, with rate constants (k) ranging from 0.0078 to 0.1549 min⁻¹ under optimized conditions. The catalyst stability and performance were examined in a reuse test, and after four cycles, the material is still greater than 60%. Thus, it was demonstrated that the presented catalysts are promising materials capable of providing feasible and useful solutions for the removal of micropollutants from contaminated water.

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O18. MOF- and ZIF-Integrated Cryogels as Monolithic Adsorbents for Water Purification: Synthesis, Characterization, and Sorption Performance

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Contamination of natural and drinking waters by heavy-metal ions and other persistent pollutants remains a priority environmental and public-health challenge, particularly in regions with intensive agro-industrial activity and aging water-supply infrastructure[1]. This creates a clear demand for sorbent materials that combine high selectivity and capacity with fast removal kinetics and practical compatibility with real water-treatment workflows. Metal–organic frameworks (MOFs) and zeolitic imidazolate frameworks (ZIFs) are widely regarded as highly promising adsorbents due to their developed microporosity, tunable node/linker chemistry, and the ability to introduce functional groups that target specific contaminants. However, real-world implementation of MOFs/ZIFs is often constrained by the “powder factor”: difficult solid–liquid separation, risks of secondary contamination by fine particles, and limited process integration into flow-through or column systems [2].

In this work, we propose a process-oriented route to convert MOF and ZIF powders into a monolithic, application-ready format through immobilization within macroporous cryogel matrices. Cryogels provide an interconnected pore network with high permeability, enabling low hydraulic resistance, efficient mass transfer, and convenient handling (shape stability, easy retrieval, and reuse). Incorporating MOF/ZIF particles into cryogels generates a hierarchical pore architecture: cryogel macropores serve as transport channels, while the micropores of the embedded frameworks supply a high density of adsorption sites. In addition, functional groups within the polymer matrix (e.g., amino, hydroxyl, and/or carboxyl groups) can enhance particle fixation and contribute to binding of target ions, improving the operational stability of the composite [3].

Hybrid cryogels are prepared by forming a polymer network via cryotropic gelation,[3,4] with following adsorption process. These strategies aim to ensure homogeneous distribution of the framework phase and robust interfacial contact between the polymer scaffold and MOF/ZIF particles critical for retaining sorption functionality under mechanical and hydrodynamic stress. Composite formation and structural features are assessed using FTIR spectroscopy(Shimadzu SpiritX), UV–Vis spectrophotometry(Shimadzu i1900), and nitrogen adsorption–desorption (BET) analysis. BET measurements quantify specific surface area and pore characteristics, while SEM-EDX enabling structure–property correlations for hierarchical porosity and chemical composition. AAS is used to determine heavy metals adsorption kinetic in model solution and real surface water, to calculate removal efficiency and adsorbent capacity.

Adsorption performance is evaluated in batch mode as a function of pH, contact time, and initial pollutant concentration, followed by data interpretation using kinetic (pseudo-first-order/pseudo-second-order) and equilibrium (Langmuir/Freundlich) models. The MOF/ZIF–cryogel composites are expected to exhibit faster uptake kinetics than the neat cryogel matrix due to high affinity of contaminant to MOF/ZIF, convective transport through the macroporous

network and rapid access to active sites within the embedded frameworks. A further performance level is selective tuning via framework choice and functionalization (e.g., amino-functionalized MOFs to strengthen coordination binding and electrostatic interactions across relevant pH windows) [4]. A key engineering advantage of the monolithic format is simplified solid–liquid separation and the potential for regeneration and multiple reuse through adsorption–desorption cycles with minimal loss of structural integrity.

From an applied perspective, the proposed platform increases the technology readiness of MOF/ZIF-based sorbents by moving from laboratory powders to a form factor compatible with flow-through purification and practical water-treatment systems. The modular nature of the approach selectable framework chemistry and adjustable polymer matrices supports scale-up and adaptation to different contaminant classes and realistic water matrices, including the presence of competing ions. In the longer term, these monolithic composites may serve as functional sorbent elements for columns, cartridges, and point-of-use devices, providing a balanced combination of high sorption performance and operational robustness.

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O19. Impact of pH, freezing temperature, and crosslinking on the transport of diclofenac sodium from freeze-dried chitosan scaffolds

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Modulated polymer-based drug delivery systems have recently gained significant popularity. Polymers combined with bioactive therapeutic agents are proven to be biocompatible, enhancing the therapeutic effects and improving release kinetics, thereby increasing system effectiveness. Polymer-based scaffolds are designed to meet the growing demand for porous and durable carriers or substrates in tissue engineering. This study aims to develop chitosan-based polymer scaffolds and investigate whether factors such as cross-linking, freezing temperature, and the pH of the dissolution medium can be used to modify their morphology and release kinetics. Freeze-dried, porous scaffolds made from chitosan were fabricated. The addition of genipin, a natural fixative, created both cross-linked and uncross-linked scaffold variations. A model drug, diclofenac sodium, was loaded into these scaffolds. The scaffolds were then tested in vitro at various pH levels to assess the impact of pH, freezing temperature, and cross-linking on the drug release profile. Compared to non-cross-linked scaffolds, those cross-linked with genipin exhibited a slower release rate of the bioactive agent. The release was more gradual in acidic media than in neutral media. The results demonstrated that cross-linking altered the scaffold's morphology and function in both acidic and neutral environments. The cross-linked scaffold could sustain and control the release of diclofenac sodium from the chitosan-based polymer scaffold, making it a promising drug delivery system.

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O20. High-, low-, and zero-spin compounds and structural variety' of 3d metals

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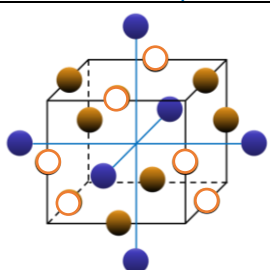
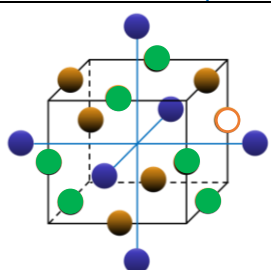
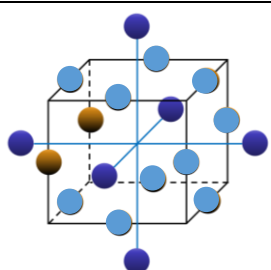
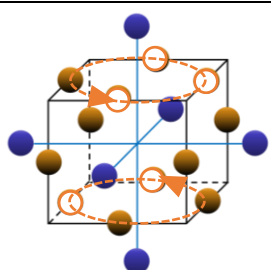
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In the presented research, the 3d structure of transition metal coordination compounds is designed using the *ID* model, which describes the structure of atomic shells using the lattice engineering technique.

Several innovative elementary theoretical concepts are introduced, such as:

- interpretation of the electron pair not as a concentration of the electron cloud on one side of the nucleus, but as a symmetric distribution of the electron cloud on both sides;
- hypothesis of the existence in the atomic shell of a new elementary particle called *magnetin*, which, by transferring the electrostatic attractive effect of the proton to the atomic shell, perform structural role as a static scheme for the forming shell, a role in chemical bonds, and in managing the energy and behavior of electrons, (*Magnetinas* are drawn as an empty circle, electrons as a filled circle);[1]
- hypothesis that electrons form atomic shells using the multilayered spatial lattice structure technique, where the dynamics between electrons and the nucleus and between the electrons themselves play specific structural roles.[2]

Tab. 1.

Statistical placement of electrons in the inner shell of iron, of cuboctahedral symmetry			
FeF ⁴⁻	Fe(CN) ₆ ³⁻	Fe(CO) ₅	FeI in metal lattices
Electrons present in the outer octahedral shell arranged for 6 electrons:			
4s ² + 4 e ⁻ acquired	4s ² + 3d ¹ + e ⁻ acquired	4s ² + 3d ⁴	4s ² free electrons
			
Electrons present in the inner shell cuboctahedral arranged for 12 electrons:			
3d ⁶ delocalized + 6 <i>magnetinas</i> = 6 e ⁻ unpaired	3p ⁶ + 3d ²⁻⁶ localized + 1 <i>magnetina</i> = 1 e ⁻ unpaired	3d ⁵⁻⁶ localized + 10 acquired from ligands = 0 e ⁻ unpaired	4 e ⁻ 3d ¹⁻⁴ localized + 2 e ⁻ 3d ⁵⁻⁶ half-free + 6 <i>magnetinas</i> = 2 e ⁻ unpaired
HIGH SPIN	LOW SPIN	ZERO SPIN	FERROMAGNETIC
Calculated magnetic spin moments (μB) [2]			
4,90	1,73	0	4,90
Observed magnetic spin moments (μB)			
5,10 – 5,70	1,73	0	2,22
Statistical spin magnetic moments calculated in the <i>ID</i> model (μB)			
≈ 5,91	1,73	0	2,83 less interaction between ordered spins

With the help of this model, which allows us to design different symmetries of atomic shells, the structural reasons for the high, low, and zero spin of the compounds and their paramagnetic and ferromagnetic properties are interpreted, as illustrated in Table 1.

Through this structural analysis, calculated and observed values of the magnetic moments of paramagnetic and ferromagnetic compounds of 3d metals and lanthanides are discussed.[3] [4]

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O21. Visible-Light-Active ZrO₂ Interfacial Charge-Transfer Complexes for Photocatalytic Hydrogen Evolution

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Zirconium dioxide (ZrO₂) is a chemically robust wide-bandgap semiconductor, but its photocatalytic activity is intrinsically limited to the UV region. In this work, we report the design of visible-light-responsive interfacial charge-transfer (ICT) complexes based on nanocrystalline ZrO₂ surface-functionalized with three organic ligands: caffeic acid (CA), 3,5-di-tert-butylsalicylic acid (di-tBuSA), and rhodizonic acid (RhA). Structural and phase composition of the ZrO₂ support was confirmed by X-ray diffraction (XRD), while X-ray photoelectron spectroscopy (XPS) verified ligand anchoring through oxygen-based functional groups and the formation of interfacial Zr–O–C bonding. Fourier-transform infrared spectroscopy (FTIR) further confirmed coordination-induced changes in carboxylate, phenolate, and quinone-type vibrations. Diffuse reflectance UV–Vis spectroscopy combined with Kubelka–Munk analysis revealed pronounced red-shifts in all three complexes. Photocatalytic hydrogen evolution was evaluated in aqueous suspensions with 2-propanol as a sacrificial agent and in situ deposited Pt as a cocatalyst. Pristine ZrO₂ exhibited only marginal activity, whereas all ICT-modified samples showed a pronounced enhancement in hydrogen production. ZrO₂/CA displayed the highest initial activity due to efficient ligand-to-metal charge transfer from catecholate groups and effective hole scavenging, although partial deactivation was observed upon prolonged irradiation. ZrO₂/di-tBuSA exhibited slightly lower but more stable hydrogen evolution, reflecting the durability of sterically protected salicylate complexes. ZrO₂/RhA showed a moderate enhancement, consistent with less efficient interfacial charge-transfer coupling.

O22. Graph-Based Machine Learning Framework for Predicting Hydrogen Storage Capacity in Metal-Organic Frameworks

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Hydrogen is a clean and high-energy fuel, yet its safe and efficient storage remains a key obstacle to widespread adoption. Metal-organic frameworks (MOFs), with their high surface area and tunable porosity, have emerged as promising candidates for solid-state hydrogen storage. In this work, we introduce a graph-based machine learning framework for predicting hydrogen uptake in MOFs by integrating spectral graph theory with data-driven modeling. Molecular structures are represented as weighted graphs from which we extract 20 graph-based descriptors, including Laplacian spectral features, degree statistics, and Zagreb indices, that capture both topological and geometric characteristics of the framework. These interpretable descriptors are used to train multiple regression models on a data set of 3300 MOFs from the Cambridge Structural Database. The XGBoost regressor achieved the highest performance in predicting hydrogen uptake, with a coefficient of determination (R^2) of 0.737, RMSE of 0.850% wt, and MAE of 0.433% wt for gravimetric uptake (UG); and a coefficient of determination (R^2) of 0.698, RMSE of 4.467 g H₂/L, and MAE of 3.045 g H₂/L for volumetric uptake (UV). Beyond accurate prediction, the framework enables inverse materials design by identifying graph-based motifs that contribute to improved storage capacity. This integration of chemical graph theory with machine learning provides a scalable, interpretable, and computationally efficient pathway for the discovery of next-generation MOFs tailored for hydrogen storage and other clean energy applications.

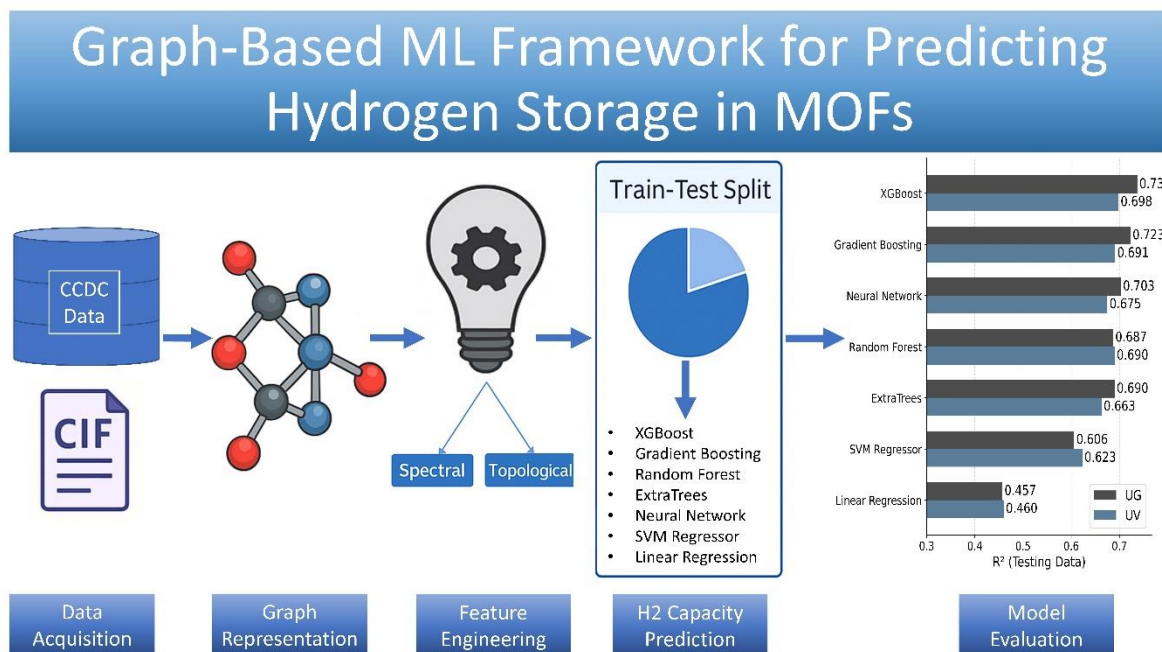


Figure 1: Overview of the proposed graph-based machine learning framework for predicting gravimetric (UG) and volumetric (UV) hydrogen uptake in MOFs. The workflow comprises (1) data acquisition from the Cambridge Crystallographic Data Centre (CCDC), (2) graph representation of MOF structures, (3) extraction of spectral and topological features, (4) training of machine learning models (XGBoost, Gradient Boosting, Random Forest, ExtraTrees, Neural Network, SVM Regressor, and Linear Regression), and (5) evaluation of predictive performance.

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O23. Novel photochromic materials for micropollutants removal

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Reactive oxygen species (ROS) play an important role in wastewater treatments processes and other biological, medical and pharmaceutical practices. Many organic compounds known also to be used as sensitizers or light harvesters able to generate ROS by direct energy transfer. Photochromic properties of ionic liquid functionalized spiropyrans have been investigated in solution and in various matrices. Especially the combination of photochromic properties and photosensitizing properties make spiropyrans highly potent compounds that are able to generate ROS. Photochromic properties of a new Fe-based highly active ionic liquid functionalized and spiropyrans functionalized nanomaterials offer an alternative method to the removal of pollutants from waters.

In this study the nanocatalysts have been synthesized, characterized and evaluated as catalysts for removal of CBZ and BPA. The ESR experiments point to an efficient formation of $^1\text{O}_2$ by the studied catalyst in aqueous suspension. The obtained recyclable photocatalysts showed enhanced catalytic behavior toward the photodegradation of selected micropollutants, due to a high yield of singlet molecular oxygen generated by active materials in the presence of UVA irradiation. Thus, the designed photocatalysts are promising nanomaterials capable of efficiently producing reactive oxygen species and removing persistent contaminants. The photocatalytic system could also be applied for the efficient degradation of a wide range of persistent, refractory and hazardous pollutants, as a pre/post-treatment sequence during the water remediation procedures.

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O24. pH-Sensitive and Antioxidant PVA–CMC Films Incorporating Eggplant Peel Extract

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Abstract

The extensive use of non-biodegradable plastics and the underutilization of food processing by-products pose significant environmental challenges. In this study, biodegradable polymer films were developed by incorporating eggplant peel extracts into a PVA–CMC matrix, transforming an agricultural waste into a value-added material. Eggplant peel, rich in phenolic compounds, flavonoids, and anthocyanins, provides strong antioxidant and antibacterial properties. Films were prepared with varying extract concentrations (0.5%, 1%, 2%) and characterized for antioxidant activity, pH sensitivity, swelling behavior, water solubility, contact angle, and structural properties using SEM and FTIR. Results indicated that films containing 2% methanol + HCl extract exhibited the highest antioxidant activity and were most suitable for food packaging applications, while 2% methanol + acetic acid extract showed the greatest swelling capacity. Most films displayed pH-responsive behavior, confirming their potential as functional, eco-friendly packaging materials.

1. Introduction

The widespread use of non-biodegradable plastic packaging and the underutilization of bioactive-rich food waste pose significant environmental challenges [1]. Polyvinyl alcohol (PVA) is produced by polymerizing vinyl acetate into polyvinyl acetate (PVAc) and hydrolyzing its acetate groups into hydroxyls, resulting in a water-soluble, film-forming, and chemically resistant polymer [2]. Carboxymethyl cellulose (CMC) is a biodegradable, water-soluble cellulose derivative with functional properties such as thickening, film formation, emulsion stabilization, moisture retention, and adhesion [3]. PVA and CMC are often combined to produce polymer films with improved mechanical strength, flexibility, water solubility, and biodegradability for packaging and biomedical applications [4]. Eggplant peel, a food processing by-product rich in phenolic compounds, flavonoids, and anthocyanins, provides antioxidant and antibacterial properties and can be valorized as a functional ingredient for food, pharmaceutical, and sustainable materials [5], [6]. This study focused on developing a biodegradable PVA–CMC polymer film by incorporating eggplant peel extract, transforming an agricultural by-product into a value-added material that not only enhances the film's functional and antioxidant properties but also supports sustainable and environmentally friendly packaging solutions.

2. Method

Eggplant peel was extracted following a modified method from Horincar G. et al. [7]. Peels (100 g) were mixed with 200 mL of either ethanol or methanol solutions containing 5% acetic acid or HCl, sonicated at 130 kHz and 70 °C for 15 min, stirred at 60 °C for 24 h, sonicated again, filtered, centrifuged at 6000 rpm for 30 min, and finally evaporated at 60 °C under reduced pressure to obtain the extracts, labelled as x (ethanol + acetic acid), y (ethanol + HCl), z (methanol + acetic acid), and t (methanol + HCl).

The film preparation followed a modified method from Kanatt S.R. [8]: 15 mL of 2.5% PVA and 15 mL of 2% CMC were dissolved separately, mixed at 70 °C for 2 h, combined, and 2% glycerol was added and mixed more 30 min. The mixture was divided into three parts, and 0.5%, 1%, or 2% of eggplant peel extracts (x, y, z, t) were incorporated and mixed more 1 h, transferred into Petri dishes, and dried at room temperature for 2 days. The films—named PVA-CMC, PVA-CMC-0.5 x/y/z/t, PVA-CMC-1 x/y/z/t, and PVA-CMC-2 x/y/z/t—were then analyzed for DPPH antioxidant activity, FTIR spectra, pH sensitivity, swelling, water solubility, contact angle, and pH-dependent colour changes. For comparison, the same film was also prepared without eggplant peel extract.

3. Results

Contact angle measurements indicated that films containing 2 % t extract were most suitable for food packaging applications. To evaluate swelling behavior, the dry weight of the films was first recorded, after which they were immersed in 20 mL of distilled water for 6 hours and reweighed. Among all formulations, the films with 2 % z extract exhibited the highest swelling capacity. pH sensitivity was assessed by applying solutions of pH 2, 4, 6, 8, 10, and 12 to the films, revealing that most of the prepared films responded to changes in pH. SEM, and FTIR analyses were conducted to examine the films' physical and chemical structures in detail. Antioxidant activity was evaluated using the DPPH assay, which showed that the films containing 2 % t extract exhibited the strongest free radical scavenging activity.

4. Discussion

Considering all test results, the 2% t film stands out as a promising material for food packaging because of its high contact angle, low water absorption, and strong antioxidant activity, providing effective functional performance while offering potential protection against oxidative spoilage and helping to extend food shelf life.

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O25. Ag, Ag₂O, and Ag–Ag₂O modified BaTiO₃/ZnO Heterostructures for Enhanced Visible-Light Photocatalysis

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Abstract

The present study reports the photocatalytic performance of Ag₂O, Ag–Ag₂O, and Ag modified BaTiO₃/ZnO heterostructures for the photodegradation of organic pollutants at the visible-light illumination. The structural, morphological, and optical features of the synthesized materials were systematically characterized to confirm the successful formation of the composites. The photocatalytic activity was evaluated through the degradation of Rhodamine B (RhB) dye [1] and the pharmaceutical pollutant paracetamol [2] under visible-light illumination. Both BaTiO₃/ZnO/Ag₂O and BaTiO₃/ZnO/Ag–Ag₂O photocatalysts demonstrated nearly-complete photodegradation of RhB. Among them, BaTiO₃/ZnO/Ag₂O showed higher adsorption capacity during the dark phase prior to illumination, which enhanced its interaction with pollutant molecules. Nearly complete photodegradation of paracetamol with BaTiO₃/ZnO/Ag₂O was also demonstrated.

Introduction

The contamination of water by organic pollutants, including dyes and pharmaceutical residues, poses a serious environmental and public health concern due to their persistence and toxicity [3]. Photocatalysis offers a sustainable approach for degrading such pollutants. However, conventional wide-band-gap semiconductors such as ZnO and BaTiO₃ are primarily active under UV light, limiting their practical use under visible illumination [4]. Modification with silver species such as Ag₂O, Ag–Ag₂O, or metallic Ag can expand light absorption into the visible region, enhance interfacial charge separation, and boost reactive oxygen species (ROS) constitution, thus augmenting photocatalytic efficiency.

Method

Silver(I) oxide (Ag₂O) was first synthesized via a precipitation method. In a typical procedure, NaOH solution was gradually added to aqueous solution of silver nitrate (AgNO₃) under continuous magnetic stirring at room temperature until pH=11–12, leading to the immediate formation of a dark brown Ag₂O precipitate. The precipitate was filtered and washed several times, then dried to obtain Ag₂O powder.

The as-prepared Ag₂O was then reduced to Ag–Ag₂O and Ag nanoparticles. Partial reduction (50%) yielded an Ag–Ag₂O composite, while complete reduction (100%) produced metallic Ag.

The obtained Ag₂O, Ag–Ag₂O, and Ag were then separately incorporated into the BaTiO₃/ZnO composite via an ultrasound-assisted self-assembly method. Components were dispersed in ethanol and ultrasonicated for 30 min. Mixtures were then dried at 120 °C to obtain the photocatalysts.

To evaluate the photocatalytic activity of the synthesized photocatalysts, photodegradation tests were performed under visible light using RhB and paracetamol.

Dispersions containing the organic pollutants and the photocatalysts were first mixed in the dark with 30 min magnetic stirrer, then photocatalysis was performed under visible light for 90 min. After separation of samples taken at specific intervals by centrifugation, residual pollutant concentrations were determined by UV-Vis spectrophotometer.

Results

XRD, FTIR, and SEM analyses confirm the successful synthesis of the nanocomposites. The reduced PL intensity of BaTiO₃/ZnO/Ag₂O, along with its lowest band gap, suggests improved charge carrier dynamics, potentially leading to enhanced photocatalytic performance.

For RhB dye, the adsorption during the dark phase was higher for BaTiO₃/ZnO/Ag₂O than for the other composites.

Direct photolysis resulted in negligible degradation of both contaminants with all photocatalysts, indicating minimal light-only effects.

In contrast, visible light illumination significantly enhanced degradation efficiency, with both BaTiO₃/ZnO/Ag₂O and BaTiO₃/ZnO/Ag–Ag₂O achieving nearly complete RhB degradation. For paracetamol, BaTiO₃/ZnO/Ag₂O demonstrated superior degradation compared to the other composites.

Discussion

The present study focuses on the photocatalytic degradation of RhB and paracetamol using silver-based materials-modified BaTiO₃/ZnO composites under visible-light irradiation. The photocatalysts were synthesized via an ultrasound-assisted self-assembly method, thoroughly characterized, and their photocatalytic efficiencies were investigated. Both BaTiO₃/ZnO/Ag₂O and BaTiO₃/ZnO/Ag–Ag₂O photocatalysts achieved nearly complete photodegradation of RhB, with BaTiO₃/ZnO/Ag₂O exhibiting a higher adsorption capacity during the dark phase. Furthermore, BaTiO₃/ZnO/Ag₂O also demonstrated nearly complete photodegradation of paracetamol, highlighting its superior photocatalytic performance and the crucial role of Ag₂O.

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O26. Effect of silver on BaTiO₃/ZnO based nanocomposites for antibacterial application

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Abstract

This study investigates the influence of silver oxidation states on BaTiO₃/ZnO-based nanocomposites for antibacterial applications. The prepared nanocomposites were assessed toward the Gram-negative Escherichia coli (E.coli) and the Gram-positive Staphylococcus aureus (S.aureus) strains. Structural and morphological analyses confirmed the successful formation of the nanocomposites, accompanied by enhanced dispersion of silver within the BaTiO₃/ZnO/Ag₂O. This composite demonstrated the lowest photoluminescence (PL) intensity, the smallest gap energy, and the highest antibacterial activity. It exhibited significantly greater antimicrobial efficiency compared to other synthesized composites and previously reported works using ZnO nanoparticles [1,2] or BaTiO₃ [3] used individually.

Introduction

The rapid emergence of antibiotic-resistant pathogens represents a critical global health challenge, driving the search for new materials that exhibit potent antibacterial activity without relying on traditional antibiotics [4]. Silver-based materials are well known for their broad-spectrum antimicrobial activity [5], and their integration into ferroelectric BaTiO₃–semiconductor ZnO heterostructures is anticipated to enhance bactericidal performance. Silver can be incorporated in different forms, such as Ag₂O, reduced Ag₂O/Ag, Ag, or Ag-doped structures and they may affect differently the antimicrobial behavior of BaTiO₃/ZnO composite.

Method

Composite materials were prepared via ultrasound-assisted self-assembly synthesis where corresponding single materials were mixed in ethanol and subjected to ultrasonic treatment for 30 min (20 sec on, 20 sec off). The solvent was subsequently removed, and mixture was dried at 120 °C.

The antibacterial activity of the synthesized nanocomposites was perused via agar diffusion method [6] toward two pathogenic bacteria: Gram-positive S. aureus (ATCC 25923) and Gram-negative E.coli (ATCC 8739). The petri dishes were then incubated at 37 °C for 24 h, and their antibacterial efficacy was assessed by measuring the inhibition zones.

Results

The XRD patterns of the synthesized composite materials exhibit the characteristic diffraction peaks of their respective individual components. The FTIR spectra also showed the main vibrational features of all constituents, confirming their successful

integration. EDX results reveal a higher surface presence of Ag in the BaTiO₃/ZnO/Ag₂O composite, while XPS analysis confirms the predominant presence of Ag⁺ species. HRTEM images display clear lattice fringes with interplanar spacings corresponding to each component.

Furthermore, the PL intensity is significantly lower for BaTiO₃/ZnO/Ag₂O compared to the other composites, indicating more efficient separation of photogenerated charge carriers within the heterojunction. This observation aligns with the band gap estimation (1.99 eV for BaTiO₃/ZnO/Ag₂O). These combined features support enhanced generation of reactive oxygen species, which are critical for bacterial inactivation, thereby strongly supporting the superior antibacterial performance of this composite.

Discussion

In this work, we directly compare the antibacterial efficacy of BaTiO₃/ZnO-based composites as a function of the type of silver species present. Among the synthesized materials, BaTiO₃/ZnO/Ag₂O exhibits the highest antibacterial activity, surpassing the other composites and highlighting the crucial role of Ag₂O in enhancing the antimicrobial performance.

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O27. Atomistic analysis of indentation-induced deformation in Nb thin films

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In this work, we explore the mechanical behavior of Niobium (Nb) using molecular dynamics simulations. The study focuses on the nanoindentation process to assess deformation defects and hardness characteristics of Nb under varying indentation velocities. The results reveal that the deformation response of the Nb specimen is influenced by the applied indentation speed. Analysis of the load-displacement curves confirms these observations: at low indentation velocities, a linear relationship indicates elastic deformation, while higher velocities result in pronounced serrations, signaling the onset of plastic deformation. Notably, the hardness remains relatively unchanged as the indenter velocity increases from 5 m/s to 10 m/s. However, a marked increase in hardness is observed when the velocity is further raised to 15 m/s.

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O28. Synthesis of green copper oxide photocatalysts for use in photocatalysis and antibacterial agents by means of plant extract

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Photocatalysis is an efficient method employed for the treatment of wastewater.¹⁻³ The CuO nanoparticle photocatalyst was synthesized via the precipitation method utilizing an extract from plant leaves.⁴⁻⁵ Its efficacy was evaluated in photocatalytic dye degradation applications. X-ray diffraction, Fourier-transform infrared spectroscopy, energy-dispersive X-ray spectroscopy, scanning electron microscopy, and ultraviolet-visible spectroscopy were employed to characterize the synthesized CuO nanomaterials.⁶⁻⁸ XRD analysis revealed monoclinic CuO nanoparticles with average crystalline sizes ranging from 25.3 to 10.5 nm. The optical band gaps ranged from 2.6 to 1.7 eV, and the FT-IR spectrum exhibited stretching vibration bands indicative of Cu-O bonds. Energy-dispersive X-ray (EDX) analysis of copper (Cu) nanoparticles elucidates their elemental composition, affirming the presence of Cu. SEM imaging reveals the morphology, dimensions, and spatial arrangement of nanoparticles. The catalytic efficacy of CuO nanoparticles infused with leaf extract was evaluated for antibacterial activity against *Escherichia coli*, *Pseudomonas aeruginosa*, and *Staphylococcus aureus*.⁹ The visible light photocatalyst, synthesized CuO (50 mg), degraded 10 ppm solutions of methylene blue, safranin, and Rhodamine 6G in water.

Keywords: Dyes, Degradation, Light, Photocatalyst, Water

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O29. Visible-Light Photocatalytic Degradation of Rhodamine 6G Using Thiourea-Derived Graphitic Carbon Nitride

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Graphitic carbon nitride ($g\text{ C}_3\text{N}_4$) was synthesized by thermal condensation of thiourea and evaluated as a metal-free photocatalyst for the visible-light-driven degradation of Rhodamine 6G (Rh6G). The as-prepared material was comprehensively characterized by FTIR, XRD, UV-Vis diffuse reflectance spectroscopy (DRS) and SEM to confirm the formation of polymeric $g\text{ C}_3\text{N}_4$, assess its band-gap characteristics and examine surface morphology. Under optimized conditions, the thiourea-derived $g\text{ C}_3\text{N}_4$ exhibited efficient Rh6G removal attributed to its suitable visible-light absorption, conjugated heptazine framework and accessible surface sites for dye adsorption and subsequent oxidative degradation. Kinetic analysis and spectral monitoring of the characteristic Rh6G absorption band demonstrated progressive decolorization with good photocatalytic stability over repeated cycles. The results highlight thiourea-derived $g\text{ C}_3\text{N}_4$ as a promising, low-cost photocatalyst for dye-contaminated wastewater treatment under visible light.

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O30. Urea-Derived Graphitic Carbon Nitride as a Catalyst for NaBH₄-Assisted Dye Reduction in Aqueous Medium

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Graphitic carbon nitride (g-C₃N₄) synthesized by calcination of urea was investigated as a sustainable, metal-free catalyst for NaBH₄-assisted reduction of organic dye in water. FTIR and XRD analyses confirmed the formation of polymeric g-C₃N₄, while UV-Vis DRS and SEM revealed its optical band-gap features and surface morphology suitable for catalytic electron transfer. In the presence of NaBH₄, the urea-derived g-C₃N₄ markedly accelerated dye decolorization, as evidenced by the rapid decay of the characteristic absorption band in UV-Vis spectra, indicating efficient catalytic mediation between the hydride donor and dye molecules. The catalyst displayed good reusability with minimal loss in activity over successive cycles, underscoring the potential of urea-derived g-C₃N₄ as a robust, low-cost material for reductive treatment of dye-laden effluents.

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O31. Melamine-Derived Graphitic Carbon Nitride for Visible-Light Degradation of Chlorophenol Pollutants

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In this work, graphitic carbon nitride ($g\text{-C}_3\text{N}_4$) obtained via direct calcination of melamine was explored as a sustainable photocatalyst for the degradation of chlorophenol under visible-light irradiation. Structural and optical characterization using FTIR, XRD, UV-Vis DRS and SEM confirmed the formation of layered $g\text{-C}_3\text{N}_4$ with an appropriate band gap in the visible region and a microstructure favourable for interfacial charge transfer. The melamine-derived $g\text{-C}_3\text{N}_4$ exhibited significant removal of chlorophenol, with the degradation efficiency governed by light intensity, catalyst loading and initial pollutant concentration. Time-resolved UV-Vis measurements indicated progressive breakdown of the aromatic ring system, consistent with hydroxyl and superoxide radical-mediated oxidative pathways reported for $g\text{-C}_3\text{N}_4$ -based photocatalysts. The study demonstrates that melamine-derived $g\text{-C}_3\text{N}_4$ provides a simple, metal-free platform for detoxification of chlorinated phenolic contaminants in water.

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O32. Thin-Film Deposition Techniques

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A solid material is said to be in thin film form when it is grown as a thin layer on a solid substrate by controlled condensation of the individual atomic, molecular, or ionic species either by physical process or ultra-chemical reactions. There are many dozens of deposition techniques[1] for material formation. Since, the concern here is with thin-film deposition methods for forming layers in the thickness range of a few nanometers to about ten micrometers, the task of classifying the techniques is made simpler by limiting the number of techniques to be considered. Most engineering materials (usually called bulk materials) have fixed properties like electrical resistivity, optical opacity, etc. Bulk materials have fixed properties and hence their applications are limited. When the thickness is reduced, beyond certain limits these properties show a drastic change. This is called size effect[2] and this adds flexibility in designing devices for a particular application. Thin film possesses attractive properties and therefore can have versatile applications. Devices with thin films occupy less space. Their fabrication requires less material, hence inexpensive.

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O33. Synthesis, Characterization, and Drug Release Profile of Cerium based Metal Organic Frameworks Loaded with Quercetin for Cancer Treatment

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Abstract

This study investigates the development of a Ce-based metal-organic framework (MOF) as a nano-drug delivery system for controlled quercetin (QUE) release. MOFs are rapidly evolving modern materials consisted of metal ions and organically coordinated molecules. QUE has been shown to have anti-cancer effects in many cancer species, including colon cancer. The Ce-QUE MOF was synthesized by dissolving Ce and H₂BDC in DMF, adding QUE, and mixing. QUE release was studied in a pH 7.4 environment. SEM analysis confirmed the microstructure, size, morphology, and porous structure of the synthesized drug delivery system, while FTIR proved the successful synthesis and drug binding. Controlled QUE release was demonstrated by UV-Vis spectrophotometry. The Ce-QUE system has the potential to develop a Ce-MOF-based drug delivery system that improves the stability, loading capacity, and controlled release of quercetin to enhance its anti-cancer efficacy.

Introduction

Metal-organic frameworks (MOFs) form a cage structure with unusual and useful properties by connecting metal-based centers to rod-like segments in a three-dimensional manner [1]. Ce ions, particularly Ce(III) ions, are plenty and low-cost rare earth elements that can be used in various biomedical implementations because of their pharmacological features, such as anticoagulant, antiallergic, anti-inflammatory, antimicrobial, antibacterial, and anticancer effects [2]. Quercetin (QUE), selected as the drug, is one of the most important and extensively studied flavonoids, found in abundance in various vegetables and fruits. QUE has been reported to exert effects on various mechanisms, including cell proliferation, angiogenesis, apoptosis, inflammation, drug resistance, cell migration, metastasis, and autophagy [3]. This study highlights its potential for controlled drug delivery systems by offering details about Ce-MOF synthesis and QUE loading/release applications.

Method

In this study, considering the Ce-MOF synthesis methods reported in the literature [4], H₂BDC was continuously stirred with a magnetic stirrer until completely dissolved in DMF. Subsequently, the mixture prepared with the Ce-containing aqueous solution was added dropwise. After ten minutes of stirring, the final mixture was placed in a Teflon-lined autoclave and heated to at 100°C for 1 hour [4]. The resulting precipitate was washed several times with deionized water and ethanol via a centrifuge at 4500 rpm and then dried at room temperature [5]. Quercetin was bound to the Ce-MOF surface

via a coordination reaction with Ce^{3+} ions. First, 100 mg of Ce-MOF was added to 30 mL of pure water and dispersed by stirring with a magnetic stirrer for 1 h. Next, 50 mg of quercetin was added to the dispersion and stirred for a further 6 hours. The resulting product was centrifuged and washed several times with distilled water, and then dried in a vacuum oven at 60°C for 12 h. The product obtained as a result of this process was named Ce-MOF/QUE. The prepared Ce-MOF/QUE was dispersed in 15 mL of PBS buffer, and the dispersion was mixed at $37 \pm 1^\circ\text{C}$ in the dark at 250 rpm. At distinct junctures, 1 mL samples were taken from the solution and centrifuged (3 min, RCF 20,000, 4°C) [6]. The synthesized drug delivery systems (DDS) were characterized via diverse methods, including FTIR and SEM. The loading and release of QUE were specified via UV-Vis spectroscopy.

Results

SEM analysis of the synthesized Ce-MOF/QUE confirmed that the porous structure was preserved before and after drug loading. FTIR spectra confirmed the synthesis of Ce-MOF/QUE and the successful binding of QUE to the Ce-MOF structure. The loading of QUE into the Ce-MOF and in vitro release behavior were characterized using UV-Vis spectrophotometry, and the controlled release profile in PBS (pH 7.4) was confirmed.

Discussion

The development of the Ce/QUE formulation for QUE drug delivery applications presents an important alternative to the literature. Ce-MOF has imparted controlled release properties to QUE. This release property has the potential to reduce the risk of side effects and increase therapeutic efficacy in pain management.

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O34. One-Pot Synthesis of Metal Nanocomposites/Graphene through Pulsed Wire Discharge

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Abstract

This study proposes a one-step, green, and low-cost route for the synthesis of graphene-based metal nanocomposites via the pulsed wire discharge (PWD) technique. Parallel-configured metal wires and graphite paper were immersed in distilled water and subjected to instantaneous high-energy pulsed discharge. Under the influence of bubble pulsations and turbulent flow, graphite flakes are effectively exfoliated while metal nanoparticles (MNPs) undergo condensation and nucleation. The resulting Cu-Sn nanoparticles/graphene primarily consists of few-layer graphene (FLG) with 3–9 layers, exhibiting a characteristic wrinkled nanosheet structure. With I_D/I_G ratios remaining between 0.12 and 0.16 at charging voltages of 20–40 kV, this physical exfoliation process preserves high structural integrity and crystallinity. The formation of M–O–C bonds ensure robust chemical anchoring of the MNPs to the graphene support.

Introduction

Graphene is widely utilized as a matrix for nanocomposites due to its exceptional thermal, mechanical, and electronic properties. Combining graphene with metal nanomaterials leverages synergistic effects to enhance overall performance. However, current research often relies on expensive pre-synthesized graphene or graphene oxide (GO), leading to high production costs and complex multi-step procedures. Pulsed wire discharge (PWD) offers a cost-effective alternative by utilizing high-density current to vaporize conductive wires into nanoparticles within nanoseconds. By using raw graphite and metal wires as direct precursors, PWD enables in-situ physical exfoliation and nanoparticle anchoring, bypassing the need for chemical pre-treatments.

Method

The pulsed discharge synthesis was conducted using a capacitor bank with a 12.5 μF capacitance and a maximum charging voltage of 40 kV. The precursors, consisting of a graphite strip (2 mm $\times$ 0.5 mm $\times$ 80 mm) and two purple copper wires (0.5 mm diameter), were arranged in parallel and fixed to electrodes using Sn solder. This assembly was immersed in distilled water and subjected to pulsed discharges at voltages of 10, 20, 30, and 40 kV.

Results

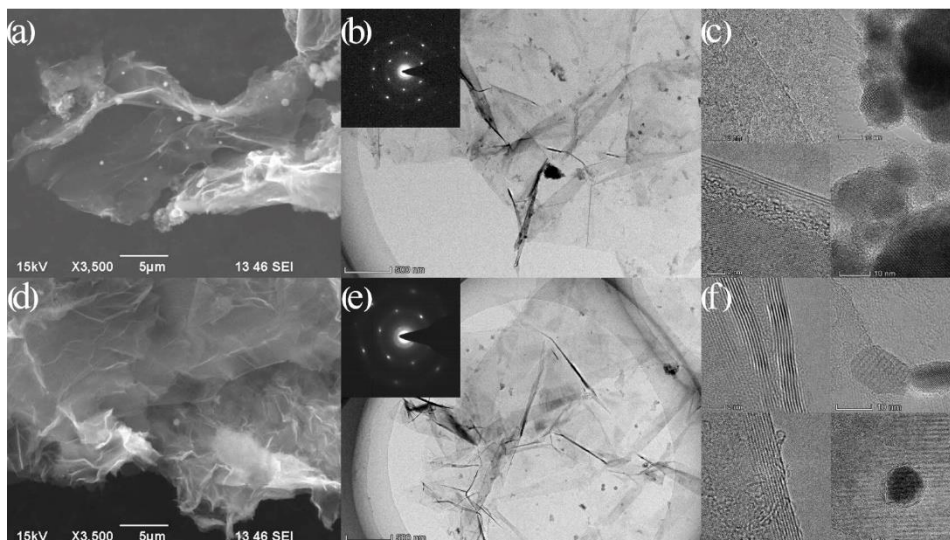


Fig. 1. (a) SEM (b) TEM and (c) HRTEM images of Sample No. 1, (d) SEM (e) TEM and (f) HRTEM images of Sample No. 3. The insets of (b), and (d) show the selected area electron diffraction patterns of Samples Nos. 1 and 3, respectively.

Morphological characterization via SEM and TEM confirmed the formation of highly wrinkled, ultrathin carbon films decorated with uniformly anchored spherical nanoparticles. Raman spectroscopy revealed I_{2D}/I_G ratios between 0.66 and 1.00, confirming the synthesis of few-layer graphene (FLG), while low I_D/I_G ratios (0.12–0.16) indicated superior crystallinity compared to chemical or electrochemical reduction methods. The crystalline structure was further validated by XRD patterns showing graphite (002) and (004) planes, with HRTEM lattice fringes matching the diffraction peaks for Sn and Cu_2O . Crucially, XPS analysis identified a peak at 532.10 eV in the O1s spectrum, corresponding to M–O–C bonds, which proves that the nanoparticles are chemically bonded to the graphene substrate rather than being physically deposited.

Discussion

The discharge process follows three stages: solid heating, liquid heating, and plasma discharge. During the plasma stage, intense shockwaves and high-temperature plasma generated by the metal wire explosion exert a violent mechanical impact on the graphite paper, leading to in-situ physical exfoliation. The metal vapor then condenses into clusters that are anchored onto oxygen-containing functional groups and defect sites on the graphene surface via chemical bonding. This unique architecture effectively suppresses the agglomeration of nanoparticles and prevents the restacking of FLG sheets, maintaining a high specific surface area for the composite material.

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O35. Synthesis and Characterization of Amoxicillin-Loaded Beta-Cyclodextrin Nanocarriers and Assessment of the Influence of Pectin Coating on Controlled Drug Release

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Abstract

In recent studies, Beta-cyclodextrin (β -CD) structures, which are nanocarriers, have attracted significant interest in drug delivery applications due to their biocompatibility, large surface area, and controlled drug release features. In this study, β -CDs were synthesized and coated with pectin (PC) to compare their stability and controlled drug release for Amoxicillin (AMX) delivery. AMX is a widely used broad-spectrum β -lactam antibiotic belonging to the aminopenicillin group, was loaded onto β -CDs, and the loading efficiency and release behavior were evaluated. β -CDs were examined using FTIR, UV-VIS and SEM to verify structural changes and drug interactions. Drug release studies under physiological circumstances (pH 7.4) were conducted to analyze the controlled release profile. The results obtained confirmed the successful synthesis of β -CDs. By demonstrating high AMX encapsulation efficiency and controlled drug release, PC-coated β -CDs have the potential to be a more effective drug delivery system compared to uncoated ones.

Introduction

Amoxicillin (AMX) exerts bactericidal activity by preventing bacterial cell wall synthesis via binding to penicillin-binding proteins, ultimately resulting in cell lysis. Despite its therapeutic effectuality versus diverse Gram-positive and Gram-negative bacteria, AMX may exhibit limited stability and rapid elimination in physiological environments, which can reduce its therapeutic efficiency. Therefore, the incorporation of AMX into nanostructured drug delivery systems has been explored to improve its stability and enable controlled and sustained drug release [1]. Nanocarriers may be a good alternative for delivering antibiotic drugs to the site of infection and ensuring their long-term and controlled release at the targeted infection site [2]. Beta-cyclodextrin (β -CD), a type of nanocarrier, is a cyclic oligosaccharide that possess a hydrophilic surface and a hydrophobic internal cavity. Studies in the literature highlight its interesting application in drug delivery systems, noting that complexation between the loaded drug and β -CD increases drug solubility and bioavailability. As an additional advantage, the entrapment

of drug molecules within the cyclic cavity of β -CD can improve drug stability and minimize drug side effects [3].

Natural polymers are widely used for drug delivery systems because of their biodegradability, biocompatibility, bioactivity, low cost, and abundant availability in nature. A popular example of a natural polymer is pectin (PC), an anionic heteropolysaccharide. The combination of rich biological activity and ionic cross-linking properties makes PC attractive for drug delivery [4].

In this study, PC-coated and uncoated AMX-loaded β -CDs were synthesized, and their structures were elucidated. Their potential as AMX transporters was comparatively evaluated through drug release studies under physiological conditions.

Method

For the synthesis of β -CD, 10 mL of 2 M KOH was first mixed in ultrapure water until dissolved. Then, 0.25 M β -cyclodextrin was added to the solution and the mixture was stirred at 500 rpm for 30 min. The acquired solution was filtered via filter paper. Subsequently, methanol was added to the solution to allow slow crystal formation by vapor diffusion, and the system was incubated at 60°C for 1 day. After, the PEG4000 solution was added to the resulting crystals to achieve a more regular morphology and nano-sized structure, and the mixture was incubated at 4°C overnight [5]. The synthesized β -CD, β -CD@AMX and β -CD@AMX@PC were characterized via diverse techniques like SEM and FTIR. The loaded and released quantities of AMX were specified via UV-VIS.

Results

To validate the successful synthesis of β -CD@AMX@PC, SEM analysis were employed to determine the nanostructure, particle size, and surface pattern. FTIR spectra were used to identify the characteristic functional groups of β -CD, PC, and AMX, and to confirm successful drug loading and PC coating. The absorption peak observed at 3417 cm^{-1} for β -CD represents to the stretching vibration of -OH involved in the intermolecular hydrogen bond within cyclodextrins, while the peaks at 2918 cm^{-1} correspond the stretching vibration of C-H in the -CH₃ and -CH₂ groups of in the hydroxypropyl structure [6]. UV-VIS analysis was used to monitor AMX loading efficiency by detecting characteristic absorption peaks. In drug loading and release studies, the amount of AMX loaded onto PC-coated/non-coated β -CDs was measured, and drug release studies were conducted under physiological conditions (pH 7.4) to investigate controlled release behavior over time.

Discussion

In this study, PC-coated and uncoated β -CDs were successfully synthesized and characterized as nanocarriers for AMX. The effects of PC coating on the controlled drug release profile were investigated. β -CDs exhibited a well-defined morphology, high drug loading efficiency, and validated PC coating. Drug release studies revealed a sustained

release profile, demonstrating the potential of PC-coated β -CDs for controlled drug delivery applications. These findings suggest that PC-coated β -CDs can serve as a promising platform for targeted drug delivery, potentially reducing systemic side effects of antibiotic drugs such as AMX and improving therapeutic outcomes. Further *in vitro* and *in vivo* research is needed to support our findings and ensure their clinical applicability.

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O36. ZrO₂@S-doped g-C₃N₄ hybrid Nanocomposites for Enhanced Dye Adsorption for MB and MO

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Graphitic carbon nitride (g-C₃N₄) was produced through high-temperature calcination of Thiourea. Its adsorption capabilities were assessed by tracking the uptake of Methylene blue and Methyl orange. The hybrids exhibited markedly higher adsorption capacity than pure g-C₃N₄ or ZrO₂. A comprehensive characterization involved X-ray diffraction (XRD), scanning electron microscopy (SEM), UV-vis diffuse reflectance spectroscopy (DRS), Fourier transform infrared spectroscopy (FT-IR) and particle size analysis (Zeta potential analysis). The ZrO₂@S-doped g-C₃N₄ hybrid nanocomposite was designed to improve dye removal through the combined advantages of its constituents. Sulfur-doped g-C₃N₄ offers a defect-rich, high-surface-area framework with abundant nitrogen sites that favor strong interaction with cationic methylene blue, while ZrO₂ contributes surface hydroxyl groups and positively charged sites that enhance adsorption of anionic methyl orange. The close interfacial integration increases available active sites, limits material agglomeration, and optimizes surface charge characteristics, leading to efficient adsorption of both dyes with good stability and reusability in aqueous systems.

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O37. Electrochemical sensing of sunset yellow with GCE/V₂O₅-rGO nanocomposite electrode

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Abstract

In this study, a new composite electrode was created by combining semiconductor-exhibiting V₂O₅ (vanadium(V) oxide) nanostructures with reduced graphene oxide (rGO). Thus, high conductivity, a large active surface area, and strong electrocatalytic performance were obtained through the synergistic effect of this composite structure. At the end of the study, a new generation sensor was developed that will enable the rapid, accurate, and reliable detection of Sunset Yellow, an artificial food coloring of critical importance for food safety.

Introduction

This study aimed to evolve an electrochemical sensor for Sunset Yellow (SSY) dye. SSY is known by the code E110 (C₆H₁₀N₂Na₂O₇S₂) and is an azo dye with a complex chemical structure. It is an important synthetic azo dye because it gives foods a yellow color and makes products more attractive. It is used in cakes, snacks, desserts, various syrups, confectionery, orange juices, and canned fish [1]. However, direct human consumption leads to serious health problems. For example, since SSY can cause health disorders such as pathogenic, allergic, and asthmatic diseases, it is important to control its concentrations [2]. The World Health Organization (WHO) has determined the daily acceptable intake of SSY as 2.5 mg/kg. However, many commercial products do not pay attention to this and use dye content in amounts exceeding the permitted limit. Furthermore, numerous European countries, particularly Norway and Finland, have banned certain synthetic colorings, such as Sunset Yellow, which are considered toxic. Therefore, accurately identifying and detecting synthetic colorings like SSY in food products appears to be extremely important and requires rapid swiftness.

Method

50 mL of H₂SO₄ and 5 mL of H₃PO₄ were added to an ice bath and the mixture is cooled to 0°C. Then, 1 g of graphite powder was supplemented and mixed with a magnetic stirrer for 10 min. 3 g of KMnO₄ was slowly supplemented to the mixture. The temperature was increased to 50°C and left to stand at a magnetic stirrer for 12 h. Then, the mixture is transferred to an ice bath, 3 mL of H₂O₂ was added, and it was washed with HCl and deionized water by centrifugation to neutralize the pH. It was dried in a vacuum oven at 60°C. The synthesized reduced graphene oxide (rGO) was characterized by FTIR and Raman techniques.

Vanadyl sulfate (VOSO₄) (0.2 mmol), iminodiacetic acid (H₂IDA) (1 mmol), and 5 ml of 0.1M H₂SO₄ were poured in a 50 mL Teflon-coated hydrothermal vat and mixed with a glass stirring rod. The Teflon-coated hydrothermal vat, which was then closed, was placed inside a pressure-resistant acid digestion vessel. It is subjected to heat treatment in an oven at 150°C for 72 h. Afterwards, the reaction vessel was taken out from the oven

and leave to cool naturally to room temperature for approximately 4 h. The synthesized V_2O_5 was washed and dried, then characterized by XRD and FESEM.

Glassy carbon electrodes (GCE) and carbon print electrodes were coated by drop method with rGO and V_2O_5 . They were dried at 80°C and made ready for electrochemical tests. Cyclic voltammetry (CV) was employed to peruse the redox mechanism of SSY on the electrode surface. Differential pulse voltammetry (DPV) was employed to detect SSY at low concentrations. Electrochemical impedance spectroscopy (EIS) was used to analyze charge transfer resistances on the electrode surface. Square wave voltammetry (SWV) was employed to analyze the effect of pH change. CV and SWV were employed to analyze the stability of the sensor to determine whether it gives the same electrochemical response over time. To determine whether the sensor specifically responds to SSY, selectivity analyzed by adding interfering ions or molecules to the SSY-containing solution and observing the change in signal.

Results

Figure 1 depicts the rGO Fourier transform infrared (FTIR) spectrum. In the spectrum of rGO, C-O (at 1052 cm^{-1}), C-O-C (at 1226 cm^{-1}), C-OH (at 1418 cm^{-1}), and carboxylic acid with carbonyl moieties at 1734 cm^{-1} and C=O indicates the presence of functional groups. For rGO spectrum, there are two peaks at 1178 cm^{-1} and 1560 cm^{-1} belong to OH groups. The Raman spectrum of rGO shown in Fig 1B. The D and G peaks are 1343 cm^{-1} and 1613 cm^{-1} , respectively. The I_D/I_G ratio of prepared rGO is 1.2. These results show that GO has been successfully reduced.

The XRD spectrum of synthesized V_2O_5 is shown in Fig. 2. When the XRD powder pattern of the synthesized V_2O_5 sample was examined, it was observed that the sample was in the orthorhombic crystal structure and indexed 98-002-9140 pattern number. No additional phases were observed in the XRD pattern. The calculate unit cell parameters of V_2O_5 a, b, c, $\alpha/\beta/\gamma$ and V are $11.4815\text{ \AA}$, $4.3624\text{ \AA}$, $3.5531\text{ \AA}$, 90° , $177.94\text{ \AA}^3$, respectively. Additionally the calculated Debye Scherrer crystalline size and microstrain are 25.48 nm and 0.795% , respectively.

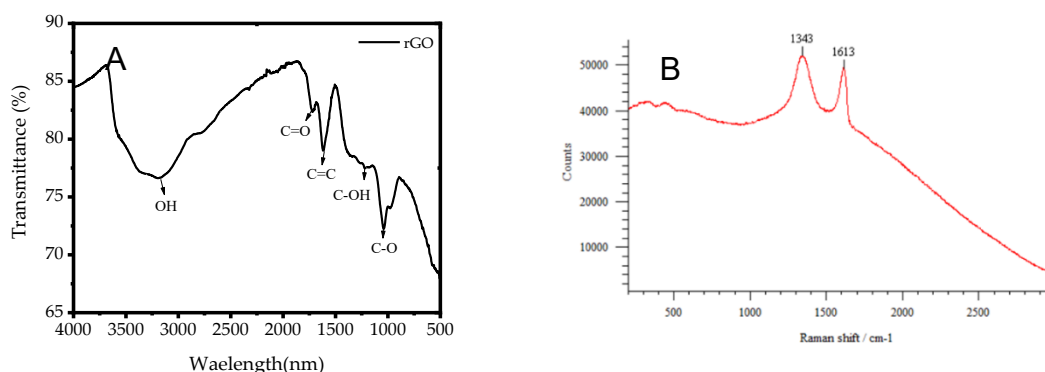


Figure 1. FTIR spectrum (A) and Raman spectrum (B) of rGO.

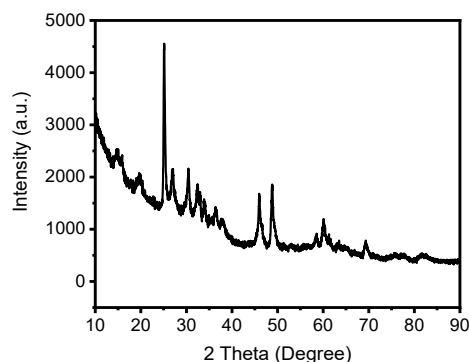


Fig. 2. XRD spectrum of synthesized V_2O_5 .

Discussion

The combination of rGO and V_2O_5 was generated a synergistic effect that enhances electrochemical sensing performance. rGO was provided high electrical conductivity and a large surface area for efficient electron transfer, while V_2O_5 was contributed strong electrocatalytic activity due to its semiconducting properties. Therefore, the rGO/ V_2O_5 composite electrode is a promising sensing material for the sensitive and reliable electrochemical detection of Sunset Yellow in food samples.

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O38. Development of MIL-101(Fe)/TiO₂ photoanode for dye sensitized solar cells

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Abstract

Solar energy is a potential alternative energy source to conventional fossil fuels. Dye-sensitized solar cells, known as 3rd generation, have found a wide field of study in recent years. In this work, TiO₂ and MIL-101(Fe) nanostructures were synthesized by hydrothermal procedure. The synthesized MIL-101(Fe) and TiO₂ nanostructures were characterized via XRD and FESEM. MIL-101(Fe)/TiO₂ photoanode prepared by the spin coating technique onto the FTO substrate. The solar cells FTO@MIL-101(Fe)/TiO₂@N719/I₃⁻/I⁺@Pt/FTO device architecture. The prepared solar cells were characterized by J-V and Nyquist curves on a 100W solar simulator.

Introduction

Recent research on dye-sensitized solar cells (DSSCs) has focused on improving efficiency, stability, and sustainability through advanced materials and device architectures. DSSCs are considered a promising third-generation photovoltaic technology due to their low cost, simple fabrication process, and efficient operation under low or indoor light conditions [1]. Current trends emphasize the development of novel sensitizers, including metal-free organic dyes and natural dyes, which enhance light absorption and reduce environmental impact [2]. Another significant trend is the exploration of advanced photoanode materials such as graphene-enhanced TiO₂ structures and bifacial DSSC architectures to improve charge transport, light harvesting, and operational stability. Furthermore, emerging approaches such as machine-learning-assisted material design and degradation analysis are being applied to optimize device performance and predict long-term stability. Overall, these advancements indicate that DSSC technology is progressing toward higher efficiency, improved durability, and broader practical applications in sustainable energy systems [4].

Method

60 mL of pure water in a beaker was mixed with 5 mL of 1 M NaOH solution. During mixing, 5 mL of titanium isopropoxide was added dropwise using a syringe, and then mixing continued for another 30 min. The resulting suspension was poured into a Teflon autoclave and treated to hydrothermal synthesis in a microwave oven at 100°C and 380 W for 45 min. The resulting TiO₂ nanoparticles were washed three times with pure water, then three times with ethyl alcohol, centrifuged at 4000 rpm, and then dried overnight in an oven at 70°C. The synthesized TiO₂ nanoparticles were characterized via XRD and FESEM by following calcination at 450°C for 3 h. For the synthesis of MIL-101(Fe), Fe(NO₃)₃·3H₂O (1 mmol) and terephthalic acid (1 mmol) were dissolved in 30 mL of deionized water and briefly sonicated to obtain a suspension with an initial pH of 2.60.

The resulting suspension was poured into a Teflon autoclave and heated in a microwave oven at 220°C and 300 W for 15 min. The synthesized MOF was washed with water, methanol, and acetone. The suspension in acetone was separated by centrifugation, transferred to N, N-dimethylformamide (20 mL), sonicated for 10 min, and stored overnight at 70°C. The acquired MOF was purified using polyvinyl fluoride and tetrabutylammonium solutions, centrifuged, repeatedly washed with methanol and acetone, and dried overnight at 75 °C. The synthesized MIL-101(Fe) was characterized via XRD and FESEM. To obtain the MIL-101-doped TiO₂ paste, 0.100 g of TiO₂ and 0.005 g of MIL-101 nanoparticles and 1 mg of ethyl cellulose were supplemented into 15 mL of ethanol and mixed for 2 h. This paste was ready for DSSC formation after sintering at 450°C for 30 min, by following the coating on FTO substrates via a glass rod. DSSCs were then generated and characterized under a solar simulator using linear scanning voltammetry to determine their electrochemical parameters (J_{sc} , V_{oc} , FF, and efficiency). The resistance characteristics and charge-transport mechanisms at the interfaces were investigated using electrochemical impedance spectroscopy (EIS). In addition, the prepared DSSCs were stored for extended periods, and electrochemical measurements were repeated at specific intervals to evaluate their stability.

Results

The XRD results of synthesized MIL-101(Fe) and TiO₂ nanostructures are depicted in Fig. 1. When the XRD powder pattern of the TiO₂ sample was examined, it was observed that the sample was in the anatase TiO₂ form and was consistent with ICDS: 98-015-4601. The peaks observed at 13.0, 16.6, 18.6, 21.6, 25.8, and 28.1 degrees in the MIL-101 Fe MOF structure belong to planes (119), (115), (004), (440), (222), and (113), respectively. The XRD powder pattern of the synthesized MIL-100 Fe MOF structures is consistent with the literature.

Examination of the FESEM images reveals that the particle sizes of the samples range from 30 to 100 nm. The particle size data agree with the crystal size values calculated from XRD powder patterns. FESEM images show that the synthesized TiO₂ powders have a tightly packed nanoporous structure. No impurities were observed in the XRD and FESEM results. In MIL-101 MOF nanostructures, aggregation in the form of nanoclusters and an average particle size of 120 nm are observed (Fig. 2B). The synthesized MOF nanostructures exhibit high surface areas and morphological features that enhance dye adhesion capacity.

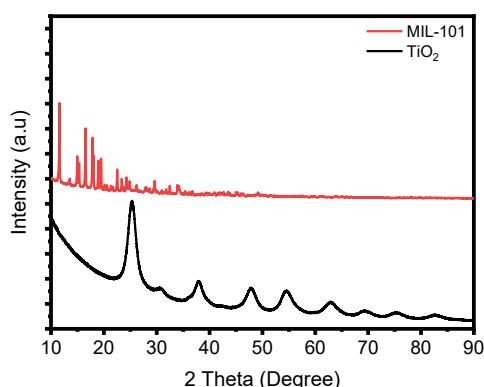


Fig. 1. XRD patterns of MIL-101 and TiO₂.

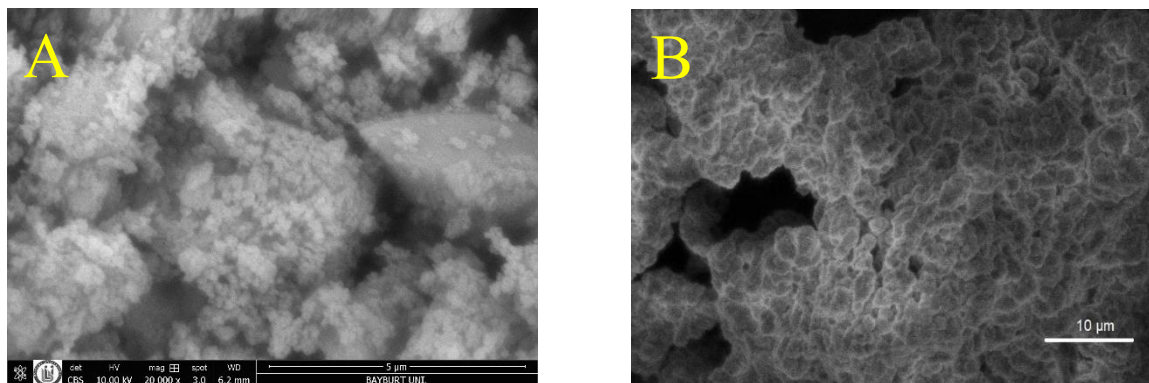


Fig. 2. FESEM images of TiO_2 (A) and MIL-101(Fe).

Discussion

This study investigated the synthesis of TiO_2 and MIL-101 MOF structures, the preparation of MIL-101/ TiO_2 paste, and the properties of solar cells. XRD and FE-SEM techniques were used to characterize the synthesized MOF and TiO_2 nanostructures. DSSCs prepared with N719 ruthenium-based dye were characterized with the help of J-V and EIS curves. The efficiency of MIL-101/ TiO_2 photoanode-based DSSC was 9.53%. Future studies will focus on investigating the stability of the developed solar cells and elucidating their mechanisms with different dye systems.

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O39. Phase Evolution and Optical Properties of Cr/Al Co-Doped BiFeO₃ Nanoparticles Synthesized via a Sol-Gel Route

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In this study, pristine BiFeO₃ and a series of Cr/Al co-doped nanoparticles with the nominal composition BiFe_{1-x}Cr_{0.5x}Al_{0.5x}O₃ (x = 0.00, 0.10, 0.20, 0.30) were synthesized via a facile citrate sol-gel route. Comprehensive characterization was performed using PXRD, Raman spectroscopy, FTIR, BET surface area analysis, SEM, and UV-Vis spectroscopy. The results revealed that increasing the dopant concentration induces a progressive phase transition from the rhombohedral perovskite structure (BiFeO₃) to the orthorhombic mullite-type phase (Bi₂Fe₄O₉).

This structural transformation was accompanied by a noticeable lattice contraction. Simultaneously, the average crystallite size decreased from approximately 46.85 nm to 28.53 nm. In parallel, the specific surface area increased significantly from 8.38 m²/g to 44.50 m²/g. Furthermore, optical characterization showed that co-doping led to a narrowing of the band gap. The optical band gap value decreased from 2.24 eV for the pristine sample to 2.05 eV for the highest dopant concentration. These findings demonstrate that Cr/Al co-doping effectively tunes the structural, textural, and optical properties of BiFeO₃-based materials. This work highlights the potential of co-doping strategies to tailor multifunctional properties in ferrite-based oxides. Overall, this study provides valuable insights for the design of advanced functional materials.

O40. BiVO₄/MWCNT composite electrodes for photoelectrochemical carmoisine detection

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- Abstract

Rapid and sensitive detection of synthetic food dyes is essential for food safety and environmental monitoring. In this study, a novel composite electrode based on bismuth vanadate (BiVO₄) and multi-walled carbon nanotubes (MWCNTs) was developed for the photoelectrochemical detection of carmoisine. BiVO₄ was synthesized via a hydrothermal method and combined with MWCNTs to enhance electron transfer and surface area. The BiVO₄/MWCNT composite exhibited superior photocatalytic activity under visible light, promoting the oxidative degradation of carmoisine on the electrode surface. Electrochemical characterization showed improved current responses and a lower detection limit compared to bare BiVO₄ electrodes. The sensor demonstrated a linear response for carmoisine concentrations ranging from 10 to 200 µM with a detection limit of 0.15 µM. The BiVO₄/MWCNT electrode combines the advantages of photocatalysis and electrochemical sensing, offering a promising platform for rapid, sensitive, and eco-friendly detection of synthetic dyes in food and environmental samples.

- Introduction

Synthetic food dyes are widely used to enhance the visual appeal of food products. Carmoisine, a synthetic azo dye, is commonly used in beverages, desserts, and processed foods; however, excessive intake has been associated with adverse health effects such as allergic reactions and hyperactivity. Therefore, its detection is crucial for food safety and regulation. Conventional methods like HPLC and spectrophotometry provide high sensitivity but require complex procedures and costly equipment [1]. In contrast, electrochemical sensing combined with photocatalytic materials offers a rapid, cost-effective, and sensitive alternative. BiVO₄ is a visible-light-active semiconductor, while MWCNTs provide high surface area and conductivity. In this study, a BiVO₄/MWCNT composite electrode was developed for photoelectrochemical detection of carmoisine [2].

- Method

BiVO₄ nanostructures were synthesized via a hydrothermal method using Bi(NO₃)₃·5H₂O and NH₄VO₃, with pH adjusted to 10–12 and treatment at 180 °C for 18 h. The obtained product was washed and dried at 80 °C. MWCNTs were purified by acid treatment (HNO₃/H₂SO₄, 1:3 v/v), washed to neutral pH, and dried. Structural and morphological characterizations were performed using XRD, FE-SEM, TEM, and Raman spectroscopy.

This study aims to develop a BiVO₄/MWCNT composite electrode for sensitive and rapid detection of carmoisine via photoelectrochemical methods. The composite structure enhances electron transfer, surface area, and photocatalytic activity. Electrochemical performance was evaluated using CV, DPV, SWV, and EIS to determine sensitivity,

detection limit, selectivity, and stability, demonstrating an efficient platform for dye monitoring.

- Results

Figure 1 The X-ray diffraction (XRD) pattern of the synthesized BiVO_4 nanostructures exhibits sharp and well-defined peaks, indicating a highly crystalline structure. All observed diffraction peaks correspond to the monoclinic phase of BiVO_4 , consistent with literature data. The most intense peak at $2\theta \approx 30^\circ$ is indexed to the (121) plane, confirming the dominant crystal orientation. Other peaks, such as (020), (110), (011), and (040), further support the phase purity of the material. The absence of additional peaks indicates that the BiVO_4 nanostructures are free from impurities and secondary phases. Overall, the XRD results confirm the successful synthesis of highly crystalline and phase-pure BiVO_4 , providing a reliable basis for further electrochemical studies and the development of $\text{BiVO}_4/\text{MWCNT}$ composite electrodes.

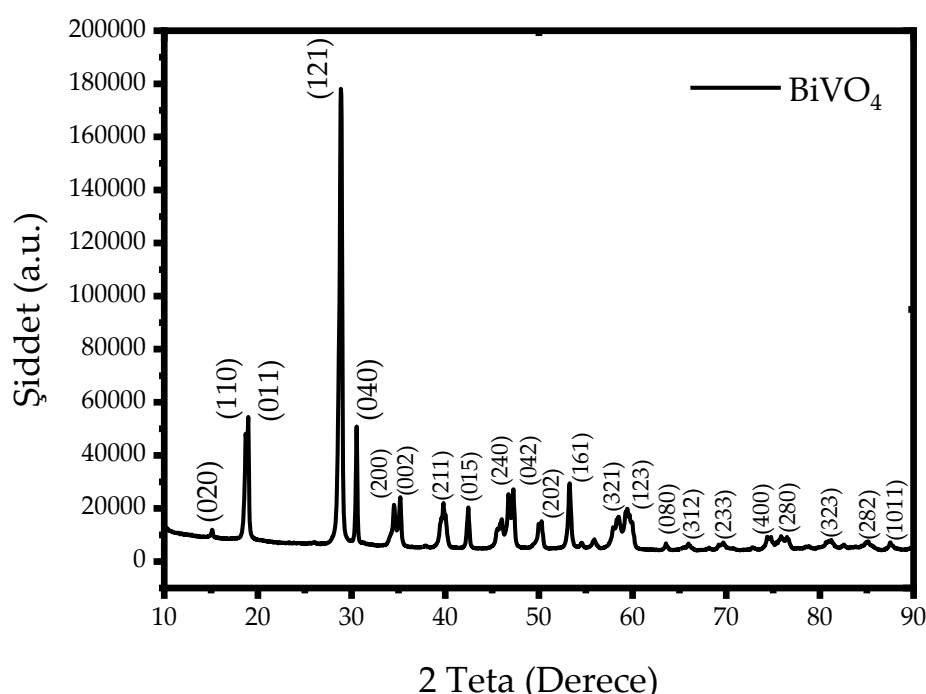


Figure 1. The XRD spectrum of prapered BiVO_4 .

The chemical structure of pristine MWCNTs was characterized by FTIR spectroscopy to identify their vibrational features. The absorption band at $1630\text{--}1650\text{ cm}^{-1}$ corresponds to C=C stretching, confirming the preservation of the sp^2 -hybridized graphitic structure. A broad band around 3400 cm^{-1} is attributed to O–H stretching, related to adsorbed moisture. Weak peaks at $2850\text{--}2950\text{ cm}^{-1}$ indicate aliphatic C–H vibrations, associated with sp^3 carbon at defect sites. Low-intensity bands in the $1000\text{--}1500\text{ cm}^{-1}$ region are assigned to carbon vibration modes. The absence of significant peaks at $1700\text{--}1750\text{ cm}^{-1}$ (C=O) confirms that the MWCNTs retain their pristine structure without notable oxidation.

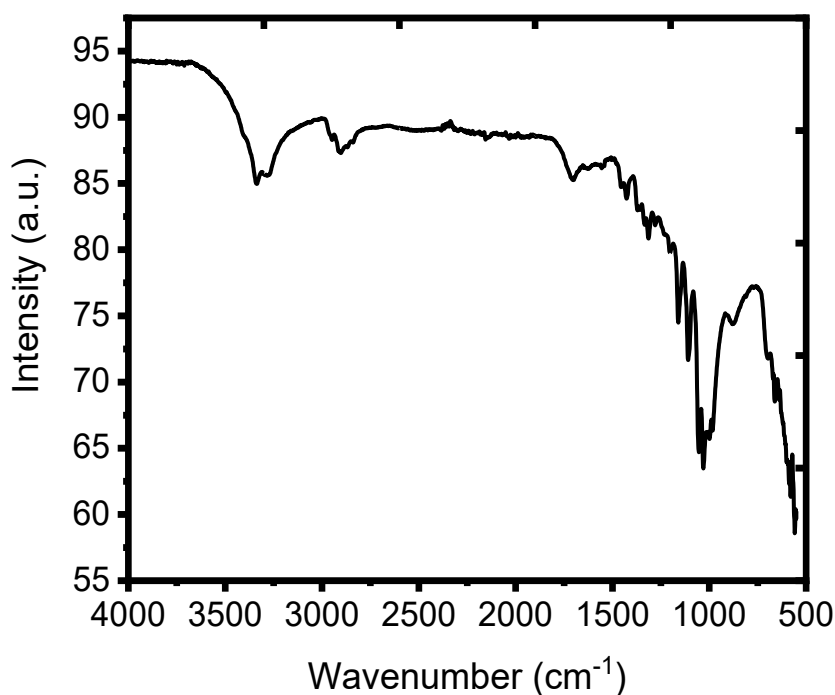


Figure 2. The FTIR spectrum of functionalized MWCNT.

In conclusion, the FTIR spectrum is consistent with the characteristics of high-purity MWCNTs. The lack of dominant oxygen-containing functional groups confirms that the structural integrity of the nanotubes was maintained during the synthesis process, providing a stable graphitic template for further applications.

- Discussion

The results demonstrate that the $\text{BiVO}_4/\text{MWCNT}$ composite electrode exhibits enhanced photoelectrochemical performance for carmosine detection compared to pristine BiVO_4 . This improvement is ascribed to the synergistic influence between BiVO_4 and MWCNTs. While BiVO_4 is a visible-light-active semiconductor, its efficiency is limited by rapid electron-hole recombination. The incorporation of MWCNTs enhances charge separation and electron transfer due to their high conductivity and large surface area. Overall, the composite electrode provides improved sensitivity and efficiency, showing strong potential for carmosine dye detection.

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O41. Transition Metal Dichalcogenides for Visible-Light Photocatalytic Degradation of Organic Pollutants - Background, Synthesis, Characterization, and Mechanistic Insights

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Abstract: Transition metal dichalcogenides (TMDs; MX_2 , $\text{M} = \text{Mo}, \text{W}$; $\text{X} = \text{S}, \text{Se}$) have emerged as potent visible-light photocatalysts for water treatment due to their tunable band structures, layer-dependent optoelectronic properties, and high density of catalytically active edge sites. Unlike wide band-gap oxides that rely predominantly on UV excitation, semiconducting 2H-MoS₂ and WS₂ exhibit strong visible absorption and suitable band edge positions for oxygen activation and hydroxyl radical generation, enabling efficient degradation of recalcitrant dyes, pharmaceuticals, and phenolics. Nonetheless, rapid charge recombination, limited basal-plane activity, and photo corrosion present critical barriers to deployment. This work integrates rational synthesis, multi-modal characterization, and mechanistic evaluation to establish design rules that translate TMD materials chemistry into durable photocatalytic performance.

Photocatalytic tests under simulated solar and visible-light irradiation demonstrate that optimized TMD heterostructures achieve accelerated degradation rates ($2\text{--}5\times$ over pristine TMDs) for methylene blue, rhodamine B, tetracycline, sulfamethoxazole, bisphenol A, and phenol at low catalyst loadings. Apparent first-order kinetics correlate with interfacial band alignment and engineered sulfur vacancies that enhance O₂ activation to $\bullet\text{O}_2^-$, while retained oxidative potential at the counter surface promotes $\bullet\text{OH}$ generation and subsequent ring-opening and demethylation pathways. Total organic carbon reduction and LC-MS tracking reveal partial to substantial mineralization with identifiable intermediates along oxidative fragmentation routes. Reusability over 5–10 cycles with minimal Mo/W leaching and preserved spectral signatures confirms structural robustness. Mechanistically, our results support S-/Z-scheme architectures that preserve strong redox endpoints while suppressing nonradiative recombination; edge/vacancy engineering amplifies adsorption and activation without triggering photocorrosion when vacancy densities are carefully bounded.

Collectively, the study advances practical guidelines: (i) maximize edge-site density via vertical alignment or controlled exfoliation; (ii) employ S-/Z-scheme junctions that maintain redox potentials and directional charge flow; (iii) introduce moderate chalcogen vacancies to activate O₂

while stabilizing the lattice; and (iv) favor earth-abundant co-catalysts with low optical losses. These insights provide a scalable pathway for visible-light-driven remediation of emerging contaminants using TMD-based photocatalysts and establish transferable principles for defect and interface engineering in 2D photocatalytic systems.

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O42. Synthesis and Characterization of Polyaniline for Photocatalytic Degradation of Organic Pollutants

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Organic polymer semiconductors play a significant role in the field of photocatalysis. In the present study, polyaniline was synthesized via chemical oxidative polymerization of aniline at room temperature. The structural and optical properties of the synthesized material were characterized by using modern analytical techniques such as X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), Scanning electron microscopy (SEM) and UV–visible spectroscopy. The photocatalytic activity of polyaniline was evaluated through the degradation of, crystal violet and safranin dyes in aqueous solution under sunlight irradiation. The results shows that polyaniline exhibits significant photocatalytic activity, demonstrating its potential as an efficient photocatalyst for water treatment applications.

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O43. g-C₃N₄ Nanocomposites for Enhanced Dye Adsorption for MB and MO

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Graphitic carbon nitride (g-C₃N₄) nanocomposites have emerged as promising adsorbents for efficient removal of cationic and anionic dyes from wastewater. Their two-dimensional structure, tunable surface chemistry, and ease of modification enable high surface area and abundant active sites for dye binding. In this work, g-C₃N₄-based nanocomposites were engineered to enhance adsorption of methylene blue (MB) and methyl orange (MO) through synergistic textural and interfacial effects. Structural characterization confirmed successful composite formation and the creation of hierarchical porosity beneficial for mass transfer. Batch adsorption studies revealed rapid uptake kinetics, with near-equilibrium removal of MB and MO within short contact times. The optimized nanocomposites exhibited markedly higher adsorption capacities than pristine g-C₃N₄, attributed to π - π stacking, electrostatic attraction, and hydrogen bonding interactions between dye molecules and functional groups on the modified surface. Isotherm analysis indicated a predominantly monolayer adsorption process well described by the Langmuir model, while kinetic data followed pseudo-second-order behavior. The adsorbents retained high efficiency over multiple regeneration cycles, demonstrating good stability and reusability. These results highlight g-C₃N₄ nanocomposites as versatile, metal-free platforms for enhanced adsorption-based treatment of MB- and MO-contaminated effluents.

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O44. Structure and relaxation dynamics in electrospun polylactide nanofibers: influence of the molecular weight

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Poly(lactic acid) (PLA) has attracted considerable attention due to its biodegradability, biocompatibility, optical transparency, and good mechanical properties, particularly a high elastic modulus and adequate strength. Owing to this unique combination of characteristics, PLA has become one of the most widely used bio-based polymers across a broad range of applications, including packaging, 3D printing, textiles, and biomedical engineering [1].

Many studies are currently exploring strategies to modify the structure of PLA in order to adjust its properties and broaden its potential uses across a wider range of applications [2,3]. In this framework, the present study aims to quantify the effect of molecular weight on the formation, morphology, and microstructure of electrospun PLA nanofibers. Three systems were investigated: High-PLA with an unusually high molecular weight (310 kDa), Medium-PLA (6 kDa), and Low-PLA (1.6 kDa).

All nanofibrous systems were systematically compared with their bulk counterparts to assess the influence of molecular weight on bulk materials and subsequently evaluate size effects associated with the nanofibrous structure. Preliminary thermal investigations performed using fast scanning calorimetry (FSC), a technique particularly well suited for nanoscale materials due to its nanogram-level sample requirement, revealed significant changes in crystallization behavior, especially for Medium-PLA. In a second part, the study focused on the influence of molecular weight on the molecular mobility of the amorphous phase, investigated through physical aging induced by structural relaxation.

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O45. *Corchorus olitorius*–Loaded PVA/PVP Hydrogels for Wound Dressing Applications

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Abstract

Hydrogel-based wound dressings are attractive biomaterials because they can maintain a moist environment, absorb exudate, and act as local carriers for bioactive compounds. In this study, physically crosslinked PVA/PVP hydrogels were prepared using the freeze–thaw method and loaded with *Corchorus olitorius* extract as a natural bioactive additive for wound dressing applications. Two loading approaches were evaluated: incorporation during hydrogel formation and loading into preformed hydrogels. The resulting systems were characterized for physicochemical and functional features related to wound care, including structural features, swelling behavior, water retention, surface wettability, antibacterial response, antioxidant activity, and model drug release behavior. The findings showed that *C. olitorius*-loaded hydrogels preserved the hydrophilic nature of the PVA/PVP matrix while exhibiting loading-dependent differences in network behavior and functional performance. Overall, the study suggests that *Corchorus olitorius* may serve as a useful natural component in physically crosslinked PVA/PVP hydrogels designed for multifunctional wound dressing applications.

Introduction

Chronic and infected wounds remain a major clinical challenge because delayed healing, excessive exudate, and microbial contamination can compromise treatment outcomes [1]. Hydrogel dressings offer important advantages in wound care due to their high water content, soft structure, and ability to support a moist healing environment. Polymer systems based on PVA and PVP have been widely explored for wound dressing design, while physically crosslinked freeze–thaw hydrogels are of particular interest because they can be prepared without conventional chemical crosslinking agents [2, 3]. In parallel, plant-derived extracts have attracted increasing attention as multifunctional additives because they may provide antioxidant, antimicrobial, and anti-inflammatory effects [3]. *Corchorus olitorius* is a widely consumed leafy plant rich in phenolic compounds, flavonoids, vitamins, and mucilaginous components, and previous studies have reported antioxidant, anti-inflammatory, antimicrobial, and wound-healing-related bioactivities for different extracts of this plant [4, 5]. Based on these properties, incorporating *C. olitorius* into a PVA/PVP hydrogel matrix may provide a simple and natural strategy for improving wound dressing functionality. Therefore, this study aimed to develop and characterize *Corchorus olitorius*-loaded PVA/PVP hydrogels and to evaluate their potential as wound dressing materials.

Method

Physically crosslinked PVA/PVP hydrogels were prepared by the freeze–thaw method. PVA and PVP solutions were first prepared separately and then mixed to obtain a homogeneous polymer blend. The hydrogel network was formed through repeated freezing and thawing cycles without the use of chemical crosslinking agents. *Corchorus olitorius* extract was incorporated by two different strategies: (i) addition to the polymer mixture before gelation and (ii) loading into preformed blank hydrogels after gel formation. The obtained samples were characterized using methods relevant to wound dressing design, including FTIR analysis, swelling and water-retention tests, contact angle measurements, morphological evaluation, antibacterial assessment against representative bacterial strains and antioxidant analysis.

Results

The freeze–thaw process successfully produced stable PVA/PVP hydrogels that can incorporate *Corchorus olitorius* extract. All hydrogels maintained the hydrophilic character expected of wound dressing, while the incorporation of extracts and the loading strategy influenced swelling, water retention, and surface behavior. Structural analyses supported the incorporation of the plant extract into the polymer matrix. Functional evaluations further indicated that the presence of *C. olitorius* contributed measurable bioactivity compared with the blank hydrogel, with antioxidant activity being more evident than antibacterial response. Overall, the results indicate that *C. olitorius*-loaded PVA/PVP hydrogels exhibit promising physicochemical characteristics for wound dressing-related applications.

Discussion

The present findings support the use of physically crosslinked PVA/PVP hydrogels as carriers for natural plant extracts in wound-related biomaterial systems. The incorporation of *Corchorus olitorius* is particularly relevant because the plant has been reported to contain bioactive phytochemicals and to exhibit antioxidant, antimicrobial, anti-inflammatory, and wound-healing activities [4, 5]. In addition, the observed differences between loading strategies suggest that the mode of incorporation influences extract distribution, surface accessibility, and overall functional response. Accordingly, *C. olitorius*-loaded PVA/PVP hydrogels may represent a useful natural-material approach for the development of multifunctional wound dressing, especially when a formulation route without chemical crosslinkers is preferred.

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O46. Development of a Self-Powered CuInSe₂/Si Photodetector

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Introduction

The potential of self-powered photodetectors (SPPDs) for energy-efficient, sustainable solutions in future optoelectronics has drawn attention in recent years [1]. Heterostructure-based photodetectors are considered a viable option in this context. One of the most well-known light-absorbing materials is copper indium diselenide (CIS), which possesses an ideal direct bandgap of 1.04 eV, a high optical absorption coefficient of 10^5 cm^{-1} , and remarkable stability [2]. Many studies have been conducted on the fabrication of photovoltaic cells using CuInSe₂ layers, but this is less explored for vertical and lateral optoelectronic sensors.

In this work, n-type CuInSe₂ thin films are prepared by thermal evaporation, and a self-powered heterojunction VIS-NIR broadband photodetector is fabricated with p-type crystalline Silicon. Here, the effect of heat treatment on various structural, morphological, optical, and electrical properties of CIS films is carefully examined. Later, a self-powered p-Si/n-CIS heterojunction device is fabricated with the CIS films treated at different temperatures.

Method

For the preparation of CIS, Cu and In₂Se₃ are co-evaporated onto the cleaned substrates after evacuating the chamber to 8×10^{-6} mbar. The precursor ratio of Cu to In₂Se₃ is fixed at 1:5 to produce near-stoichiometric films. Both the deposition and annealing temperatures are varied to examine the impact of temperature variations on the absorber film. The substrate temperature is first set to 300°C, and samples 300A, 400A, and 300S show how the annealing temperature is increased from 300 to 500°C in 100 °C increments. The substrate temperature is adjusted in 100°C increments from 300 to 500°C after the annealing temperature is fixed (samples 400S and 500S). For device fabrication, n-type CIS films subjected to different temperature treatments are coated onto p-Si to form p-n heterojunction photodetectors.

Results

The X-ray diffraction pattern of the as-deposited film suggests its amorphous nature. Upon annealing, all the films become polycrystalline with a preferential orientation along the (112) plane, matching well with the tetragonal structure of CIS (JCPDS No. 00-040-1487). As the temperature treatment increases, the crystallite size increases and the dislocation density decreases. Similarly, Raman spectra confirm the formation of CIS, with the intensity of the A1 mode increasing with heat treatment, indicating improved crystallinity. The variation in surface morphology with different deposition temperatures is studied in detail. The as-deposited films appear homogeneous and uniform. Increasing the temperature promotes grain coalescence, leading to larger clusters. This can be attributed to the substantial increase in thermal energy, which leads to greater mobility and diffusion, in turn resulting in nucleation and island formation. The morphological variation with respect to annealing temperature suggests that annealing promotes grain growth and defect elimination, such as grain boundaries. Hall measurements confirm the

n-type conductivity of the films and the drastic decrease in resistivity with the temperature treatment.

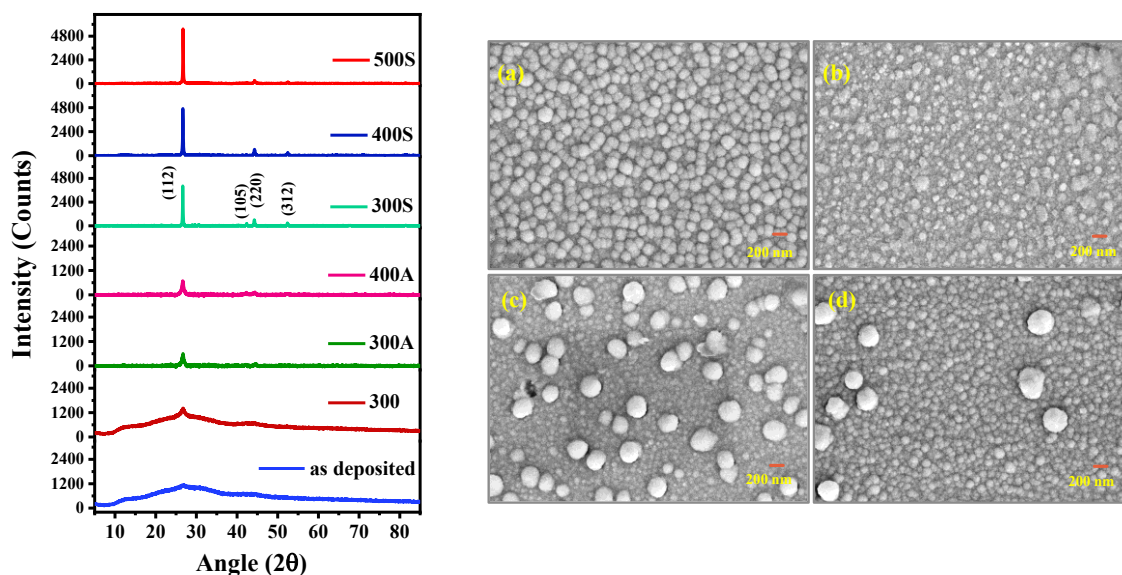


Fig 1(a). XRD patterns of CIS films (b) SEM images of (a) as-deposited film and films with substrate temperature (b) 300 (c) 400 (d) 500 °C

Si/CIS-3A, Si/CIS-4A, Si/CIS-3S, Si/CIS-4S, and Si/CIS-5S are the labels of the heterojunction devices using 300A, 400A, 300S, 400S, and 500S CIS layers, respectively. The device's current-voltage (I-V) characteristics are recorded in both dark and light conditions to assess its potential for self-powered operation. All the devices have shown a rectifying behavior. The sample treated at the highest temperature exhibits a notable increase in photocurrent when compared to the sample annealed at the lowest temperature. Due to the built-in potential at the Si/CIS-5S junction, the device exhibited an open-circuit voltage of 94 mV and a short-circuit current of 3.4×10^{-5} A.

The photosensitivity of the Si/CIS-5S device is 128 times higher than that of the Si/CIS-3A device. The Si/CIS-5S heterojunction achieves its maximum responsivity at zero bias, with a value of 8.22 mA/W. Similarly, the Si/CIS-5S heterojunction has the highest detectivity of 6.21×10^{10} Jones, due to its strong responsivity and reduced dark current. The Si/CIS-5S device demonstrated the best performance as a self-powered photodetector, with the highest responsivity, detectivity, and ON-OFF ratio.

For further device analysis, the spectral responsivity of the Si/CIS-5S device is measured over the 300-1100 nm wavelength range. At 940 nm, the EQE spectrum produced a maximum value of around 13.6%, which corresponds to a peak spectral responsivity of 0.10 A/W. With a peak value of 2.34×10^{12} Jones at 940 nm, the detectivity likewise exhibits notable improvement throughout the entire spectrum. Due to simultaneous photodetection in the Si and CIS films, the device exhibited significant photon-to-electron conversion in the near-IR range. To ensure practical feasibility, the device's stability is crucial. The long-term continuous photoresponse, various switching responses, and device ageing are examined to assess this. By sustaining its photoresponse in all these conditions, the detector demonstrated remarkable stability.

Discussion



CuInSe₂ thin films are prepared using single stage thermal evaporation technique. Pre- and postdeposition thermal treatments at 300 °C and 500 °C resulted in a film with higher crystallinity. Both the photosensitivity and electrical characteristics of the absorber layer improved when the CIS layer was treated with a high substrate and high annealing temperature. The enhancement of crystallinity, the elimination of grain boundaries, and the decrease in resistivity observed in the XRD, SEM, and Hall measurements, respectively, further support these results. The heterojunction's photoresponse can be efficiently adjusted by thermal treatment of the CIS layer.

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O47. Comparative Study of N₂ and H₂S Annealing on Grain Growth and Surface Morphology of CZTS Thin Films

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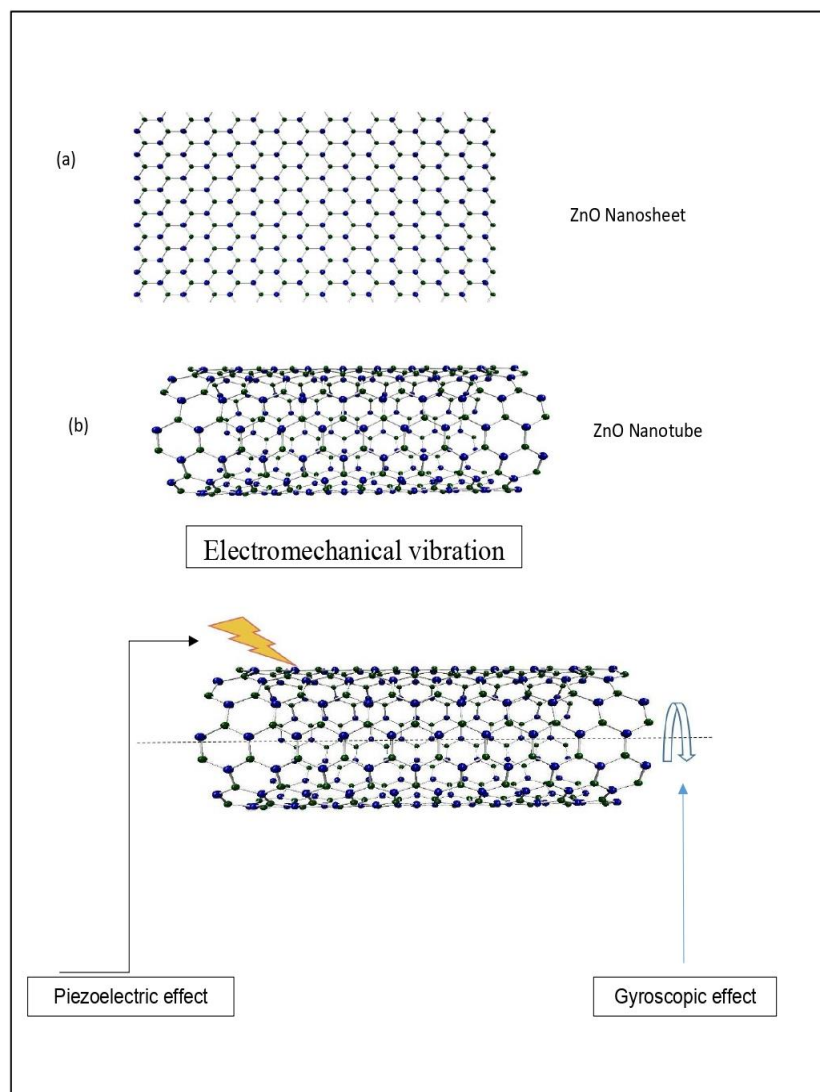
Solar cells convert sunlight into electricity via the photovoltaic effect and are a promising solution to the global energy crisis. In this study, CZTS (Cu₂ZnSnS₄) thin films were grown using a single-step electrodeposition method for PV applications. Deposition was carried out at -1.05 V (vs. Ag/AgCl) for 30 minutes on a molybdenum (Mo) substrate in a three-electrode electrochemical cell, with bath pH maintained at 5. A platinum (Pt) plate and Ag/AgCl electrode were used as the counter and reference electrodes, respectively. Two sets of samples were obtained by annealing the as-deposited CZTS thin films at 550 °C for 30 minutes under N₂ and H₂S atmospheres, respectively. The surface morphology and photoelectrochemical (PEC) performance of as-grown, N₂-annealed, and H₂S-annealed CZTS thin films were systematically investigated using scanning electron microscopy (SEM) and current-voltage (I-V) measurements. The as-deposited films exhibit a relatively smooth yet non-uniform surface with no clearly distinguishable grains, indicating poor crystallinity and an amorphous or poorly developed structure. Correspondingly, the I-V characteristics reveal no observable photoactivity under PEC conditions, which can be attributed to high defect density and inefficient charge separation. Upon annealing in a nitrogen (N₂) atmosphere, discernible grains emerge with an average size of approximately 717 nm, suggesting enhanced atomic diffusion and partial recrystallisation. This morphological improvement leads to a slight increase in photoactivity compared to the as-grown films; however, the films remain somewhat non-uniform, with voids and agglomerations indicating incomplete densification due to the absence of sulfur, thereby limiting their PEC performance. In contrast, films annealed in an H₂S atmosphere demonstrate a significant enhancement in both morphology and photoresponse, exhibiting a dense, compact, and uniform surface with well-defined larger grains averaging ~912 nm. The corresponding I-V characteristics show clear p-type photoconductivity, with V_{oc} of approximately 204 mV and a J_{sc} of about 114 μA cm⁻² under identical PEC conditions. This pronounced improvement is attributed to the sulfur-rich environment, which promotes enhanced crystallization, proper kesterite phase formation, and reduced sulfur vacancy defects. While N₂ annealing provides moderate improvements, H₂S annealing is essential for producing highly crystalline, dense CZTS films with significantly enhanced PEC performance for photovoltaic applications.

O48. Piezoelectric and spin effects on the vibration behavior of spinning SWZnONTs

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Owing to their remarkable piezoelectric and magnetic characteristics, single-walled zinc oxide nanotubes (SWZnONTs) are considered promising candidates for rotating elements in nanoelectromechanical systems (NEMS). In this work, the vibrational behavior of a rotating SWZnONT subjected to electrical loading is investigated. To accurately account for size-dependent and electromechanical coupling effects, the formulation incorporates nonlocal strain gradient theory along with Maxwell's electrostatic relations. The nanotube is modeled as a Timoshenko beam, and the governing equations together with the associated boundary conditions are derived using Hamilton's principle. The resulting equations of motion are solved through a Galerkin-based analytical approach, allowing the determination of the vibration response of the rotating smart nanotube. Furthermore, a parametric study is carried out to evaluate the influence of key factors, including the material length scale parameter, nonlocal effects, rotational speed, applied voltage, and boundary conditions, on both the natural frequencies and the critical rotational speed.



O49. Modification of the Physical and Chemical Properties of Biomaterials Derived from Sol-Gel Technology

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Abstract: Hydroxyapatite (HAP, $\text{Ca}_{10}(\text{PO}_4)_6\text{OH}_2$) bioceramic, titanium dioxide (TiO_2) ceramic, and stainless steel are biomaterials widely used in biomedical applications. In this study, we investigated the effect of combining HAP and TiO_2 phases on the surface of a 316L stainless steel substrate, using the sol-gel deposition process, on the properties of the resulting material. The sol-gel method enabled the formation of thin coatings adhering to the substrate at an annealing temperature of only 500°C, corresponding to the crystallization temperature of hydroxyapatite. The HAP sols and gels were characterized to evaluate their composition and the evolution of their microstructure throughout the aging process. The addition of TiO_2 to the hydroxyapatite phase increased the uniformity of the coatings and thus reduced surface roughness. Consequently, reinforcing the HAP coating with TiO_2 significantly improved its adhesion strength to the substrate. Furthermore, immersion testing of the HAP/ TiO_2 materials in a physiological solution demonstrated improved properties in terms of chemical stability and resistance compared to pure HAP.

Introduction

Among all the bioceramic materials based on calcium phosphate (CaP) currently in use, hydroxyapatite (HAP) is the most commonly used as a bone substitute due to its favorable biological and physical properties [1]. However, the low mechanical strength of HAP limits its practical applications to situations requiring little or no load. Consequently, to expand the scope of HAP's application to sites subjected to significant loads, such as dental or hip implants, a composite system comprising an HAP coating [2] on a biocompatible metal implant [3] has been used. Furthermore, the addition of metallic elements such as titanium (Ti) or its oxide to the HAP coating could improve the coating's hardness [4]. Thus, the objective of this work is to study the effect of combining HAP and TiO_2 phases on the adhesion strength of the layer deposited on the substrate, as well as the corrosion resistance and chemical stability of HAP/ TiO_2 materials in physiological solution. HAP and TiO_2 were synthesized using a sol-gel process that enables the preparation of various high-quality HAP-based bioceramic materials [5-7]. Controlling the stability of sol-gel solutions in terms of aging time is necessary to develop the desired solid structures. Insufficient aging can lead to the formation of secondary phases other than hydroxyapatite, or of other non-stoichiometric phases, which can be attributed to an incomplete reaction between the various precursors [8]. The adhesion of the coating was estimated using a scratch test.

The chemical stability and residence of the materials was tested in the simulated body fluid (SBF) solution. The interaction between the physiological environment and the material in contact was studied using atomic absorption spectroscopy and potentiodynamic cyclic voltammetry test. Additionally, the microstructural properties and morphological characteristics of the sol-gel-synthesized materials were examined.

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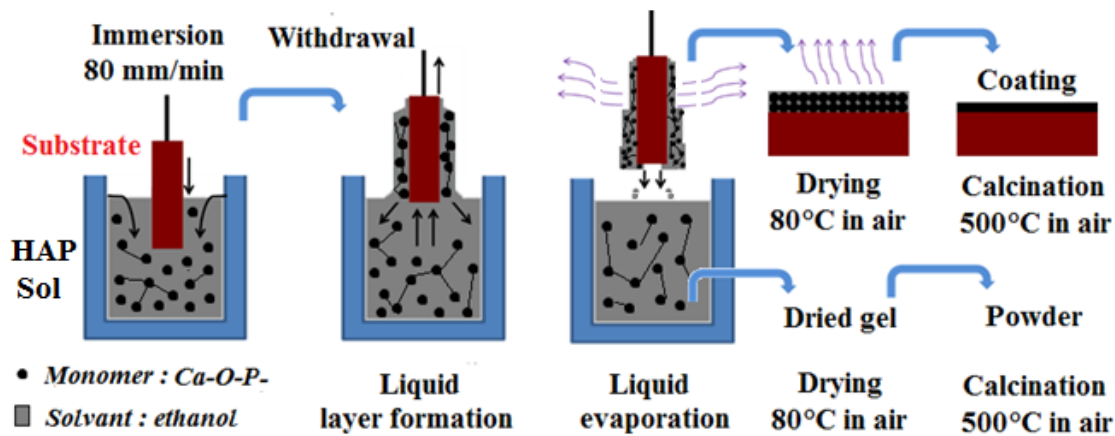


Figure 1: Main steps of the sol-gel process.

O50. Engineering solar-driven systems for sustainable water treatment through low-dimensional materials

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Nanomaterials have become a highly relevant area of research due to their unique mechanical, chemical, and optical properties, as well as their nanoscale dimensions.[1] These characteristics, together with their high specific surface area, make them ideal for numerous applications in fields such as biomedicine, electronics, and photocatalysis.[2]

The development of heterostructures combining organic and/or inorganic nanomaterials has gained increasing attention in recent years. These systems aim to integrate complementary properties while overcoming the intrinsic limitations of individual components.[3] Traditionally, such heterostructures relied on weak van der Waals interactions, which often limit their stability under harsh chemical or thermal conditions. In contrast, recent advances in covalent bonding strategies have enabled the fabrication of more robust and versatile architectures, leading to improved performance in applications such as energy storage, catalysis, sensing, and electrochemistry.[3] Therefore, covalently engineered nanomaterial heterostructures represent a promising platform for the design of advanced functional materials.

In this work, we focus on photocatalysis, addressing the critical challenge of maximizing visible-light utilization to enhance solar-to-chemical energy conversion, improve charge separation, and increase pollutant adsorption. To this end, we develop a covalently engineered low-dimensional heterostructure by integrating a two-dimensional material (MoS₂) with zero-dimensional carbon dots, aiming to achieve enhanced stability and photocatalytic efficiency for sustainable water treatment applications.

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O51. Covalent Engineering of Transition Metal Dichalcogenides: From Molecular Design to Hybrid Heterostructures

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The unique physical properties of two-dimensional (2D) materials have placed them at the forefront of materials science, yet translating these properties into functional technologies often demands precise chemical control over their surfaces. Covalent functionalization offers a direct route to modulate the electronic structure, reactivity, and interfacial behavior of these layered systems, and among available strategies, maleimide-based chemistry has proven especially effective for the selective modification of transition metal dichalcogenides (TMDs), enabling molecular-level design of hybrid nanomaterials with tailored properties. [1]

A key advance in this direction is the development of bifunctional molecular bridges carrying orthogonal reactive handles. This strategy makes it possible to covalently link TMDs to other 2D platforms, yielding chemically interconnected heterostructures whose properties are no longer limited by weak van der Waals interactions. [2] The resulting covalent junctions provide enhanced thermal and mechanical stability alongside electronic characteristics that are largely governed by the molecular nature of the interlayer connection. [3] The same synthetic logic further enables the construction of vertical homostructures with programmable interlayer spacing, a parameter of direct relevance to optoelectronic performance through its influence on interlayer coupling. [4]

Here we present an overview of these covalent approaches, emphasizing clickchemistry-based protocols applied to TMD platforms. We highlight how rational molecular design at the interface opens realistic pathways toward multifunctional 2D architectures that surpass the capabilities of conventional non-covalent assemblies.

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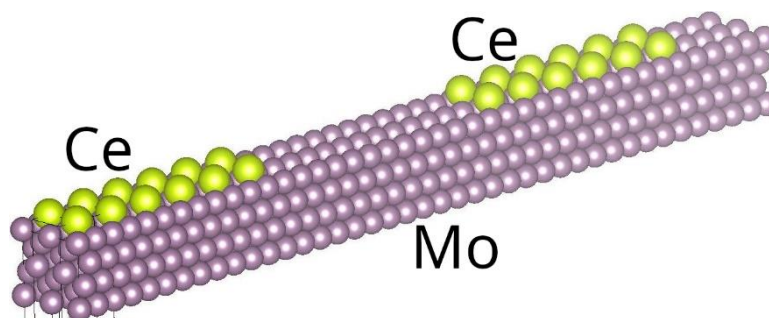
O52. Nanometer Scale 2D Structures in Cerium + Oxygen Submonolayer Films on Mo(112) Surface: Experiment + Theory

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Cerium and oxygen adsorbates on the Mo(112) substrate were shown to form a rich variety of ordered super-structures in the coverage range up to a single monolayer [1-2]. Experimentally, low energy electron diffraction (LEED) had been used to uncover the symmetry and spatial periodicity of the formed super-structures. Due to a highly anisotropic furrowed structure of the Mo(112) substrate and the intricacies of the inter-adsorbate and adsorbate-substrate interactions, some very long unit cells are formed within the Ce+O admixtures, the longest reported one reaching 40 times in-plane [111] periodicity of Mo(112).



Understanding physics behind such super-structures' nature and stability requires *ab-initio* modeling of large periodic slabs containing hundreds of atoms. This often sets prohibitively enormous requirements on the computing resources if performed with the help of plane wave based computer codes implementing the density functional theory approach. However, atomic orbitals based codes, in particular SIESTA, which was specifically designed to handle system sizes on the order of thousand atoms, allow such simulations on modern computer hardware. We report on SIESTA simulations of the structures reported in [1-2] and compare them to our experimental results.

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O53. Optimizing Process Parameters for Nanomachining of Lithium Niobate

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Lithium niobate (LN) remains a cornerstone material in modern photonics, valued for its exceptional electro-optic, nonlinear optical, and piezoelectric properties. Despite its utility, standard nanofabrication techniques—such as focused ion beam milling and electron beam lithography—often involve prohibitive costs and complexity, particularly for rapid prototyping and small-scale development. This study proposes Atomic Force Microscopy (AFM)-based nanomachining as a highprecision, cost-effective alternative for the fabrication of LN optical waveguides.

The primary objective of this research is to characterize the nanomachining behavior of LN by systematically investigating the influence of critical process parameters, including optimal loading force, tip velocity, and number of machining cycles. Through this investigation, we establish the specific machining conditions required to achieve targeted feature depths while minimizing surface roughness. Reducing roughness is paramount in waveguide fabrication to mitigate optical scattering losses and enhance the efficiency of electro-optic field interactions. The results provide a strategic framework for utilizing AFM nanomachining as a viable pathway for the iterative prototyping of high-performance photonic components.

O54. Preliminary Study on Thermal Quenching-Induced Exfoliation of Vein Graphite using HCl Acid Medium

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Graphite exhibits enhanced functionality upon exfoliation, which disrupts ordered layering, increases interlayer spacing, and introduces partial structural disorder. Among the exfoliation methods, thermal quenching is a rapid and efficient method that induces stress within the graphite structure by heating, followed by sudden cooling. However, systematic studies on the influence of acid concentration during quenching remain limited. In this study, Sri Lankan vein graphite, notable for its high purity and crystallinity, was subjected to thermal quenching using HCl as the quenching medium. HCl was selected due to its non-oxidizing nature, relatively low toxicity and ability to facilitate intercalation and protonation. Graphite rods (2.5 x 1.5 x 0.5 cm) were heated at 800 °C for 1 h and quenched in HCl solutions of varying concentrations (0.10, 0.25, 0.50, 0.75 and 1.00 M) followed by sonication, neutralization, drying and dispersion.

X-ray diffraction indicates the slight increase in interlayer spacing from 3.3468 Å (raw graphite) to 3.3539 Å, 3.3554 Å, 3.3598 Å, 3.3563 Å and 3.3531 Å, respectively for samples quenched in 0.10, 0.25, 0.50, 0.75 and 1.00 M HCl solutions, while preserving the overall crystalline structure. Fourier Transform Infrared spectroscopy analysis confirmed intercalation and protonation, with minimal oxidative functionalization, indicating preservation of the aromatic framework. Particle size analysis revealed that the 0.75 M HCl-quenched sample exhibited the lowest polydispersity, whereas other concentrations showed broader particle size distribution. The highest carbon content (96.26%) was observed in the 0.1 M sample, indicating minimal oxidation and contamination. These findings confirm that thermal quenching in HCl enables controlled, partial exfoliation of vein graphite while preserving its crystallinity. This approach holds potential for producing graphite materials suitable for electronic and energy storage applications. Further, studies could explore alternative quenching media to optimize exfoliation efficiency and material performance.

O55. Magnetic TiO₂/Carbon Quantum Dots nanocomposites as sustainable photocatalysts for antibiotic removal from water

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Water scarcity combined with the increasing presence of pharmaceuticals, such as antibiotics, in aquatic systems poses a significant threat to environmental integrity and human and animal health. The increasing demand for efficient and sustainable materials for water treatment has driven research towards photocatalytic technologies. In this work, magnetic TiO₂/Carbon Quantum Dot (CQD) nanocomposites were synthesised and evaluated to assess the influence of synthesis methodology on the final material's photocatalytic performance. CQDs were synthesised via a hydrothermal method using spent brewery grains (SBGs) as a sustainable carbon precursor. The process involved hydrothermal carbonisation at 200 °C, with or without prior stirring at 70°C of the precursors, followed by filtration and purification. Magnetic TiO₂/CQDs nanocomposites were then prepared via co-precipitation of iron salts, either in situ or ex situ, enabling facile recovery of the materials by means of magnetic separation. For the ex situ methodology, TiO₂/CQD nanocomposites were previously prepared through ultrasonication, followed by co-precipitation with iron oxide. In the in situ synthesis, CQDs, TiO₂, and iron salts were added together. Four magnetic TiO₂/CQDs composites were obtained by combining stirring and the synthesis route (in situ or ex situ).

The prepared materials were evaluated for the photocatalytic degradation of 10 mg/L trimethoprim (TMP) and sulfamethoxazole (SMX) in phosphate buffer (0.001 mg/L, pH 8) under simulated solar irradiation. The results show that all nanocomposites enhanced the degradation of both TMP and SMX compared to photolysis. The best-performing photocatalysts removed more than 70% of antibiotic after 1 h of irradiation, compared to less than 20% removal in photolysis. Under the tested conditions (500 mg/L), the ex situ photocatalyst with prior stirring exhibited the highest activity, yet the results were comparable to the in situ photocatalyst without prior stirring, which was selected as the most suitable photocatalyst due to simpler and faster synthesis. Subsequently, its photocatalytic performance was optimized by testing different catalyst loadings and further investigated in a mixed solution of TMP/SMX. The effects of pH, radical scavengers, and humic acids were evaluated to further understand the degradation mechanisms, and the photocatalyst was finally tested in a real wastewater matrix, confirming its potential for practical application in antibiotic removal.

O56. Gyroscopic Effects in Rotating Functionally Graded Nanotubes: An Exact Analytical Study

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This paper investigates the rotordynamic behavior of spinning functionally graded nanotubes (FG-NTs), with particular emphasis on the gyroscopic effect. Equations of motion are derived using Hamilton's principle within the framework of Euler-Bernoulli beam theory and nonlocal elasticity, with the gyroscopic effect rigorously incorporated into both the differential equations and boundary conditions—an aspect overlooked in several prior studies. The coupled equations are uncoupled via a complex displacement transformation, cleanly separating forward and backward whirl motions. The state-space method provides exact natural frequencies for four classical boundary conditions: Clamped-Clamped (C-C), Clamped-Simply Supported (C-S), Clamped-Free (C-F), and Simply Supported-Simply Supported (S-S). The influences of nonlocal parameter, material gradient index, and length-to-diameter ratio on both forward and backward whirl frequencies and critical speeds are systematically studied.

O57. Influence of Material Gradient Index and Composition on the Vibrational and Dynamic Properties of CNT/SiCNT Functionally Graded Nanotubes

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This study examines the role of material composition and gradient distribution in determining the dynamic behavior of functionally graded nanotubes (FG-NTs). The FG-NT is designed as a hybrid nanostructure combining an outer carbon nanotube (CNT) layer—providing exceptional structural rigidity—with an inner silicon carbide nanotube (SiCNT) layer offering superior thermal insulation properties, ideal for fluid-conveying or high-temperature nanodevice applications. Material properties including Young's modulus and density are graded continuously through the nanotube wall thickness according to a power-law distribution controlled by the gradient index n . The effect of n on natural frequencies and critical speeds is studied under Eringen's nonlocal elasticity and Euler-Bernoulli beam theory, solved exactly using the state-space method. Results demonstrate that the gradient index governs a transition from CNT-dominated (stiff, high frequency) to SiCNT-dominated (compliant, low frequency) behavior, with distinct sensitivity regimes separated at $n \sim 1$. The interplay between material gradient, nonlocal parameter, and boundary conditions is characterized in detail.

O58. Eco-Friendly Biopolymer-Based Hydrogels for Controlled Water Release in Sustainable Agriculture

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The agricultural sector is currently facing major challenges due to rapid population growth and increasing pressure on natural resources. Water scarcity is one of the most critical constraints for sustainable agricultural production. Against this backdrop, the development of eco-friendly materials has emerged as a promising strategy for enhancing water management in agriculture.

This research project focuses on synthesising and characterising biopolymer-based hydrogels as eco-friendly materials designed to release water in a controlled manner in soil under various hydric stress conditions. These hydrogels are made from natural polysaccharides that are biodegradable, non-toxic, renewable, cost-effective and environmentally sustainable. The physicochemical properties of the synthesised hydrogels, particularly their swelling behaviour and water retention capacity in soil, are characterised. These properties make the hydrogels highly efficient at enhancing soil moisture and reducing water loss.

Overall, this work contributes to the development of sustainable, environmentally friendly hydrogel systems with controlled-release properties, offering a promising solution for improving water use efficiency and supporting sustainable agriculture.

O59. Formulation of Biopolymer-Based pH-Responsive Indicator Films for Smart Food Packaging

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The need for packaging solutions that not only maintain food quality but also take into account environmental limitations and changing consumer expectations is growing in the modern food sector, especially in Mediterranean nations. Intelligent and environmentally friendly packaging that can minimize food loss, cut down on plastic waste, and give real-time freshness information is becoming more and more necessary.

This study explores the formulation and evaluation of pH-sensitive biofilms developed from renewable biopolymers, specifically carboxymethyl guar, chitosan, xanthan and related systems. These biopolymers are selected for their biodegradability, safety, and compatibility with food systems, as well as their potential to valorize locally available agrosources. The films are enriched with natural colorimetric indicators, such as anthocyanins extracted from plant sources, which exhibit visible color changes in response to pH shifts caused by food degradation.

The mechanical performance, barrier effectiveness, and pH sensitivity of the prepared films are evaluated. To ascertain their applicability as freshness indicators in actual food-packaging settings, structural investigations, optical characterisation, and colorimetric stability tests are carried out. These films can lessen food waste, a major problem for Mediterranean supply chains, by increasing shelf life and facilitating early spoiling detection.

All things considered, this work advances the creation of next-generation active and intelligent food packaging materials that combine social impact (better food safety and consumer confidence), economic potential (valuation of local resources and potential cost reduction through waste minimization), and environmental sustainability (biodegradability, reduced plastic use). This is consistent with current initiatives in the Mediterranean agrifood industries that support circular and sustainable packaging solutions.

O60. Engineering of new biobased hydrophobic polymers for slow release fertilizer: Formulation and agronomic assessment

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The increasing demand for sustainable agricultural practices has catalyzed the development of environmentally friendly fertilizer delivery systems. This study focuses on the synthesis, characterization, and agronomic evaluation of innovative ethyl cellulose (EC)-coated controlled-release NPK fertilizers, enhanced with novel bio-based plasticizers derived from fatty acids present in waste cooking oil. These plasticizers, including esters, epoxides, and polyols, were synthesized through a multi-step process involving transesterification, epoxidation, and subsequent functionalization, converting low-value waste oils into effective plasticizing agents compatible with EC matrices.

The incorporation of these plasticizers into EC films significantly improved their mechanical flexibility, film-forming ability, and controlled permeability, addressing the limitations typically associated with pure EC coatings. Comprehensive characterization techniques—including thermogravimetric analysis (TGA), tensile testing, dynamic mechanical analysis (DMA), and scanning electron microscopy (SEM)—were employed to evaluate the structural and thermal behavior of the modified films. Release kinetics studies revealed that the plasticized EC coatings enabled sustained nutrient release, effectively reducing leaching and improving nutrient use efficiency.

Agronomic trials under both greenhouse and field conditions demonstrated that the plasticized EC-coated fertilizers enhanced soil moisture retention, improved nutrient availability, and led to a notable increase in crop yield compared to conventional uncoated fertilizers. This research highlights the potential of valorizing waste-derived fatty acids to create biodegradable and efficient fertilizer coatings, offering a promising solution for climate-smart and resource-efficient agriculture.

O61. Ni-Assisted Densification and Electrochemical Characterization of $\text{BaCe}_{0.7}\text{Zr}_{0.1}\text{Y}_{0.1}\text{Yb}_{0.1}\text{O}_{3-\delta}$ Proton-Conducting Ceramics

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The worldwide transition toward sustainable energy technologies has driven growing interest in intermediate-temperature solid-state systems, including protonic ceramic cells and electrochemical reactors for environmentally friendly ammonia production. Among the electrolyte materials under investigation, $\text{BaCe}_{0.7}\text{Zr}_{0.1}\text{Y}_{0.1}\text{Yb}_{0.1}\text{O}_{3-\delta}$ (BCZYYb) is particularly promising because of its outstanding proton conductivity. Nevertheless, the large-scale fabrication and commercialization of BCZYYb-based devices remain challenging, mainly due to the very high sintering temperatures (1600–1700 °C) needed to achieve proper densification. This work examines the role of Ni as a sintering aid in lowering the densification temperature of BCZYYb without compromising its functional performance. BCZYYb powder, prepared via the glycine–nitrate combustion method, were impregnated with 0 to 8 mol% Ni^{2+} and sintered over a temperature range of 1300–1600 °C.

Dilatometric measurements together with SEM/EDS characterization showed that the incorporation of only 1 mol% NiO markedly changes the sintering behavior, allowing higher densification and a uniform microstructure at lower sintering temperatures than those required for NiO-free and commercial BCZYY reference materials. Phase development and structural stability were investigated by temperature-dependent XRD, while thermogravimetric analysis verified the material's ability to incorporate protons, evidenced by a characteristic mass loss between 450 and 700 °C attributed to dehydration.

To assess how Ni addition influences transport behavior, electrical conductivity was analyzed by AC impedance spectroscopy with porous Pt electrodes under different atmospheres (air and 10% H_2/N_2 , in both dry and humid conditions). In addition, Faradaic efficiency measurements of both BCZYYb and the optimized BCZYYb/Ni ceramics were carried out between 300 and 600 °C to evaluate their performance under practical operating conditions.

Acknowledgements: This work was carried out within the framework of the ALCHEMHY project (no. 101177996), funded by the EU Horizon Europe Research and Innovation Actions programme, and the project CICECO – Aveiro Institute of Materials (UID/50011/2025, LA/P/0006/2020, UID/PRR/50011/2025), financed by national funds through FCT/MCTES (PIDDAC).

O62. Approaches for recovery and reuse of nickel from end-of-life high-temperature fuel cells

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The growing demand for sustainable materials in advanced electrochemical energy conversion technologies, such as molten carbonate fuel cells (MCFCs) and solid oxide fuel cells (SOFCs), underscores the urgent need for effective recycling strategies. This study explores approaches for the recovery and reuse of nickel from spent MCFC and SOFC stacks.

For MCFCs, the recycling strategy involved mechanical grinding of the stack followed by selective dissolution of carbonates using acetic acid, enabling the separation of nickel from potassium and lithium carbonates. The process parameters were optimized using the Taguchi method, allowing the identification of conditions that improve efficiency while reducing reagent consumption and processing costs.

In the case of SOFCs, the recycling approach was based on redox treatments under varying redox cycles to promote cathode delamination, enabling the recovery of the remaining Ni-YSZ structure. The remaining parts were ground and ball-milled for reuse in SOFC anodes.

Ni-YSZ cermets and symmetrical YSZ cells with Ni-YSZ electrodes were developed using reference materials to evaluate electrical conductivity and electrode polarization resistance, respectively. These systems serve as benchmarks for future comparison with electrodes and cells fabricated using recycled nickel.

Preliminary results demonstrated the feasibility of reusing recycled materials in the manufacture of functional electrodes, with performance metrics comparable to those of conventional counterparts. The findings lay the groundwork for further optimization of the recycling protocol, with the goal of enabling more sustainable and cost-effective fuel cell fabrication.

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O63. Relaxation dynamics of poly(lactic-co-glycolic) acid nanocomposites

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Understanding the structural organization of nanocomposites is essential to tailor their properties for the targeted application. This means elucidating how nanofillers are distributed within the polymer matrix and how this distribution governs the material properties. Indeed, the concentration and spatial arrangement of nanofillers play a critical role in both the ageing behavior of the material [1] and its mechanical performance [2], among others. In the case of lamellar nanofillers, three morphologies are primarily observed: (i) the fillers form agglomerates with little influence on chain dynamics, (ii) they intercalate between polymer chains, inducing confinement effects, or (iii) an exfoliated morphology is achieved when dispersion is optimal, leading to peculiar properties related to the filler/matrix interactions [2]. When these interactions are promoted, the glass transition dynamics are modified. In particular, the size of the cooperative rearranging region (CRR) increases, as evidenced by several studies [3].

In this study, the relaxation dynamics of nanocomposites are investigated in poly(methyl methacrylate) (PMMA) and poly(lactic-co-glycolic) acid (PLGA), filled with black phosphorus nanolayers (2D-bP). In a first time, the thermal stability of the nanocomposites was assessed by thermogravimetric analysis coupled with Fourier transform infrared spectroscopy (TGA-FTIR). Then, the glass transition was probed by modulated temperature differential scanning calorimetry (MT-DSC), enabling the calculation of the CRR size using Donth's method [4]. Finally, fast scanning calorimetry investigations allowed to investigate the relaxation dynamics related to the glass formation and to extract the fragility index [5].

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O64. Analysis of Two-Dimensional and Three-Dimensional Heat Conduction in Composite Thermal Storage Materials

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Abstract: This study investigates the characteristics of two-dimensional (2D) and three-dimensional (3D) heat conduction in composite thermal energy storage materials based on Phase Change Materials (PCM), consisting of paraffin, ice pack, and zeolite. The primary objective is to analyze temperature distribution, heat flux behavior, and thermal energy storage capacity of the composite wall system under tropical environmental conditions. A numerical approach based on the Finite Volume Method (FVM) is employed and integrated with experimental temperature measurements obtained at multiple points, including the upper surface, internal layer, lower surface, and ambient environment. An effective thermal conductivity value of 0.90 W/m·K is used to represent the homogenized behavior of the heterogeneous composite system. The results indicate that the 3D model provides a more realistic representation of temperature distribution compared to the 2D model, particularly in capturing volumetric thermal gradients. Furthermore, the composite material demonstrates significant thermal damping behavior, characterized by reduced temperature amplitude and time lag relative to ambient temperature fluctuations. These findings highlight the potential of PCM-based composite materials for energy-efficient building applications in tropical regions.

Introduction

Energy efficiency in buildings has become a critical issue due to the increasing global energy demand and the need for sustainable development. One promising approach to improve thermal performance in buildings is the application of Phase Change Materials (PCM), which can absorb and release large amounts of heat during phase transitions [1]. The integration of PCM into building envelopes, particularly in wall structures, has been widely recognized as an effective strategy to enhance thermal stability and reduce cooling loads [2].

However, most previous studies have primarily focused on single PCM materials such as paraffin or salt hydrates, which often exhibit limitations in terms of thermal stability, heat distribution, and long-term performance [3]. To overcome these limitations, composite PCM systems combining multiple materials have been proposed. In this study, a hybrid composite consisting of paraffin as the primary latent heat storage medium, hydrogel-based ice pack as an initial cooling enhancer, and zeolite as a porous stabilizing material is investigated [4]. Despite the growing interest in such composite systems, studies that integrate experimental analysis with two-dimensional and three-dimensional numerical modeling remain limited, particularly under real tropical environmental conditions characterized by high temperature fluctuations [5]. Therefore, this research aims to

analyze heat conduction behavior in composite PCM materials using both experimental and numerical approaches [6], [7]. The study focuses on understanding temperature distribution in 2D and 3D models, evaluating heat flux characteristics based on measured data, and assessing thermal energy storage performance and thermal damping effects within the composite system [8].

Method

The composite material used in this study consists of paraffin as the primary phase change material, hydrogel-based ice pack to enhance cooling performance, zeolite as a porous stabilizing medium, and concrete brick as the structural matrix. The thermophysical properties applied include a density of 1800 kg/m^3 , a specific heat capacity of $840 \text{ J/kg}\cdot\text{K}$, and an effective thermal conductivity of $0.90 \text{ W/m}\cdot\text{K}$, representing the homogenized behavior of the heterogeneous composite system. The wall thickness is defined as 0.065 m . Temperature data are obtained experimentally using sensors placed at four key locations: the upper surface, internal layer, lower surface, and ambient environment. Measurements are recorded at regular time intervals to capture transient thermal behavior and are used to validate the numerical model [9].

The numerical analysis is based on the transient heat conduction equation, solved using the Finite Volume Method. The two-dimensional model evaluates temperature distribution on a planar domain, while the three-dimensional model accounts for volumetric heat transfer, including spatial variations in all directions [10]. Heat flux is calculated using Fourier's law based on the temperature difference across the wall, while thermal energy storage is evaluated from the internal temperature variation relative to the initial condition [11], [12].

Result

The results show that the 2D model produces a nearly linear temperature gradient across the wall thickness, indicating dominant one-dimensional conduction behavior. In contrast, the 3D model reveals non-uniform temperature distribution within the composite, especially near edges, highlighting the importance of multidimensional heat transfer. The heat flux follows ambient temperature variations, with peak values occurring at maximum temperature differences between the upper and lower surfaces. The composite PCM material reduces peak heat flux and enhances thermal energy storage, as reflected by the stabilized internal temperature profile.

Discussion

The comparison indicates that while the 2D model is suitable for simplified analysis, the 3D model provides a more accurate representation of real thermal behavior due to its ability to capture volumetric effects. The combination of paraffin, ice pack, and zeolite enhances thermal performance through latent heat storage, improved heat distribution, and delayed temperature rise. The observed reduction in temperature fluctuations and heat flux confirms a strong thermal damping effect, which is beneficial for maintaining

indoor thermal stability. These results demonstrate the potential of composite PCM materials for energy-efficient building applications, particularly in tropical environments.

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O65. Finite Volume Method in Heat Transfer Process in Paraffin, Zeolite and Ice Pack Based Brick Composites

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Abstract: This paper presents an ICNMSME 2026 manuscript template prepared from the uploaded experimental dataset for a composite brick thermal storage system containing paraffin, zeolite, and ice pack. The work focuses on the application of the finite volume method (FVM) to describe transient heat transfer behavior and on the evaluation of one-dimensional conductive heat flux through the brick section. The analysed dataset consists of 49 measurement points collected at 15-minute intervals from 06:00 to 18:00, including upper-surface temperature, internal brick temperature, lower-surface temperature, ambient temperature, FVM output, model error difference, and heat flux. The temperature history shows that the external surface reached a maximum of 45.52 °C, while the brick core reached 44.58 °C, indicating a moderated thermal response inside the composite body. The computed FVM variable ranged from 14.79 to 26.37 with an average value of 22.24. The heat flux profile varied from negative values in the late afternoon to a peak positive value of 64.38 W/m² at 10:00, revealing strong diurnal heat penetration and subsequent reversal. The results confirm that the paraffin-zeolite-ice pack composite brick is able to delay and attenuate heat transfer, although the model error trend indicates that additional calibration of effective thermal properties is still required. This template is organized according to the ICNMSME paper format and can be directly expanded with author identity, final references, and deeper validation results.

Introduction

Heat transfer through building envelopes is a primary challenge in tropical climates. This study investigates a composite brick (batako) integrating paraffin (latent storage), zeolite (thermal buffer), and an ice pack (cooling capacity) to enhance thermal inertia. Using a one-day transient dataset, the material's thermal response is analyzed via the C and experimental heat flux estimations. Structured as an ICNMSME-ready template, this paper covers the background, methods, results, and conclusions, requiring only final author details and bibliography for completion. [1-5]

Method

The dataset contains 49 time steps recorded every 15 minutes (06:00–18:00, 26 Dec 2025) to analyze the composite brick's daytime thermal behavior using various temperature, FVM, and heat flux measurements. The numerical model employs a 1D Finite Volume Method (FVM), discretizing the brick and using the transient conduction.

Result

The observation revealed a clear transient heating process: the outer surface peaked at 45.52 °C (12:15), while the internal temperature peaked later at 44.58 °C (13:45).

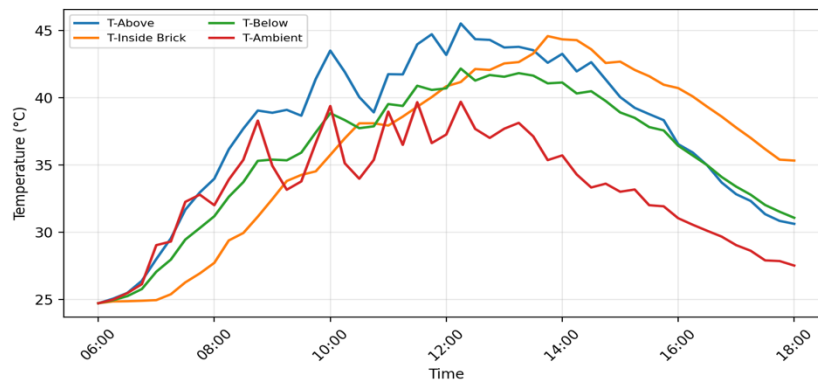


Figure 1. Temperature profiles of the composite brick system from 06:00 to 18:00. The FVM model captured this conduction trend with an average error of 14.15. Additionally, the conductive heat flux reached a maximum of 64.38 W/m^2 at 10:00 before reversing to -9.43 W/m^2 at 17:30.

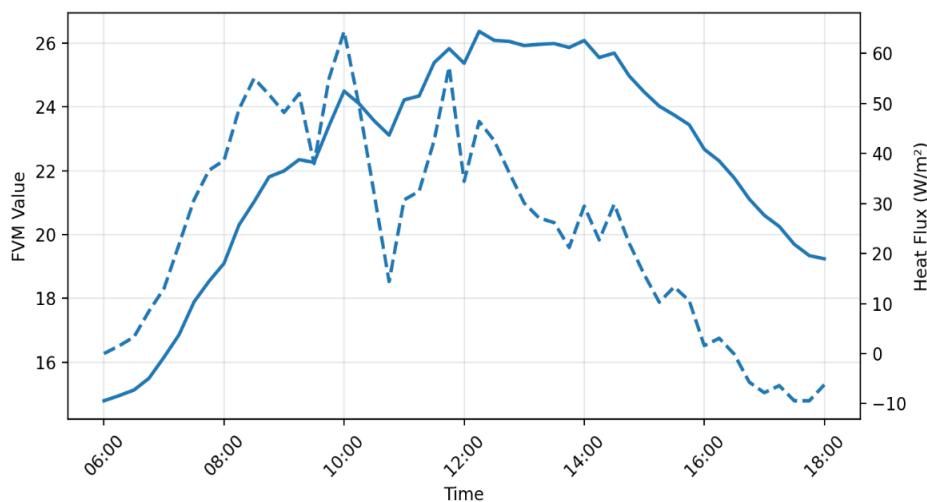


Figure 2. Comparison between finite volume method output and conductive heat flux.

Discussion

The delayed response between the outer and internal temperature peaks confirms the composite brick's ability to attenuate and store heat. Furthermore, the reversal of the heat flux to a negative value demonstrates that stored heat is effectively released during the cooling stage. Although the FVM model captured the general conduction trend, the observed average error indicates that further parameter calibration is still needed. Overall, the composite brick effectively attenuates and stores heat, providing adequate preliminary results for the ICNMSME paper. Future studies should focus on further model calibration and statistical validation.

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O66. Experimental Study of Energy-Efficient Wall Using Hybrid PCM (Paraffin, Ice Pack, and Zeolite) Under Tropical Climate Conditions

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Abstract: Energy consumption in buildings continues to be a significant concern, especially in tropical areas where elevated ambient temperatures and solar radiation markedly heighten cooling requirements. This study experimentally examines the thermal performance of a building wall incorporating hybrid phase change materials (PCM) comprising paraffin, hydrogel-based ice pack, and natural zeolite. An outdoor experiment was set up in real tropical conditions to look at temperature profiles, thermal energy storage, and thermal buffering. The results show that the hybrid PCM wall has more thermal inertia, less temperature change, and a longer time for heat to move than regular walls. The system could store up to 1.93 MJ/m² of thermal energy, and the buffer energy could be anywhere from 1009 kJ/m² to -701 kJ/m². There was a time difference of about 90 minutes between the outside surface and the wall core, which shows that the thermal buffering was very good. These results show that hybrid PCM systems are a good way to passively cool energy-efficient buildings in tropical climates.

Introduction

The building sector uses more than 30% of the world's energy and produces nearly 40% of its carbon emissions [1]. This problem is especially important in tropical areas, where high solar radiation and ambient temperatures make cooling needs much higher because air conditioning is used so much [2]. In equatorial areas like Pontianak, Indonesia, solar exposure stays pretty much the same all year, which means that building envelopes, especially walls, keep getting hotter all the time. Walls are the main way that heat gets into indoor spaces [3]. Phase change materials (PCM) have been extensively researched as passive thermal energy storage systems owing to their capacity to absorb and release latent heat during phase transitions [4]. Prior research has shown that the incorporation of PCM into brick materials can diminish heat transfer and enhance thermal stability [5], [6], [7]. Nevertheless, the majority of studies concentrate on individual PCM systems within regulated laboratory settings, exhibiting restricted validation in authentic outdoor contexts [8]. To fill this gap, this study suggests a hybrid PCM system that uses paraffin, a hydrogel-based ice pack, and natural zeolite. This combination of latent and sensible heat storage with better structural stability is meant to improve thermal performance in tropical conditions [9], [10]. The study empirically assesses temperature distribution, time delay, thermal energy storage, and buffer energy properties.

Method

The composite wall is modelled as a uniform medium with an effective thermal conductivity of $0.90 \text{ W/m}\cdot\text{K}$, which is the same as how the heterogeneous material system would behave [7]. The wall sample was made to be $132 \text{ cm} \times 61 \text{ cm} \times 6.5 \text{ cm}$ so that heat would mostly move in one direction. The hybrid PCM was made up of 40% paraffin, 30% ice pack, and 30% zeolite. The materials were melted, hydrated, and mixed together before being put into the wall core. The experiment took place outside in the sun. Every 15 minutes, thermocouples recorded the temperature data.

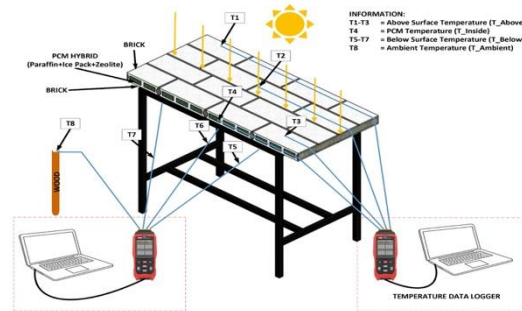


Figure 1.

Experimental setup

We figured out how much thermal energy could be stored per square metre by looking at the composite wall's sensible heat capacity. Buffer energy, on the other hand, was the difference in temperature between the wall core and the outside air. These parameters were utilised to assess the thermal storage and buffering efficacy of the system [8].

Results

The results show that the hybrid PCM wall works well in hot weather. The temperature in the room went up from 25°C to almost 40°C . The outer surface reached its highest point at 45.52°C and the wall core reached its highest point at 44.58°C , with a 90-minute delay. This shows that heat was absorbed well and transferred slowly.

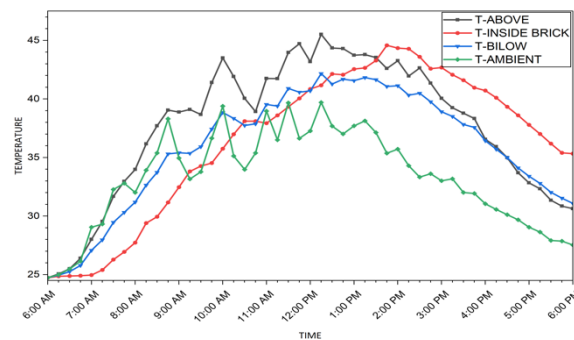


Figure 2. Temperature profile vs time

The temperature difference was 3.35°C , which showed that the heat was being effectively reduced. The wall core's delayed peak shows that there is thermal inertia from phase change and the interaction of hybrid materials. When heating, thermal energy storage went up to a maximum of 1.926 MJ/m^2 , showing that it can hold a lot of heat.

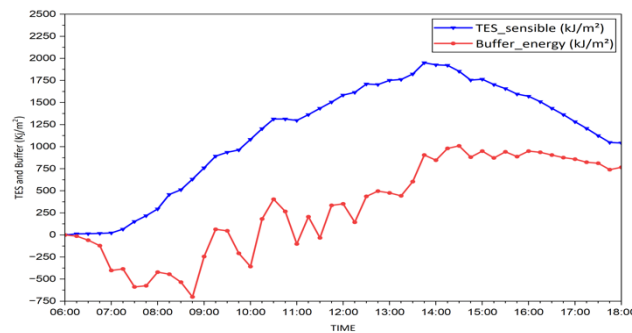


Figure 3. Thermal energy storage and buffer energy vs time

Buffer energy has both positive and negative values, which means that heat is moving around. The wall core's maximum temperature of 1009 kJ/m² shows that it was hotter than the surrounding air, while the minimum temperature of -701 kJ/m² shows that it was cooler than the surrounding air, confirming that the wall acted as a thermal buffer.

Discussion

The findings validate that the hybrid PCM wall enhances thermal efficiency via the integration of latent and sensible heat storage. The 90-minute time lag shows that the material has a lot of thermal inertia, which is in line with what other studies of PCM-integrated bricks have found [5], [6]. The increased thermal energy storage shows that it can absorb heat well during times of high solar radiation. Paraffin provides latent storage, the ice pack helps with transient cooling, and zeolite improves stability and conductivity. Buffer energy analysis shows dynamic heat exchange, where positive values mean heat release and negative values mean heat absorption. This behaviour shows that the system acts as a thermal buffer, which helps keep the temperature stable and makes the indoors more comfortable [7], [8], [9], [10].

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O67. Controlled Hydrothermal Growth of Hollow CoS₂ Microspheres as High-Performance HER electrocatalysts

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CoS₂ nanoparticles were synthesized using a simple hydrothermal method, and their structural, optical, and chemical features were thoroughly examined with XRD, UV-DRS, FTIR, FE-SEM, and EDX analyses. Their electrochemical behaviour was further evaluated through CV, GCD, EIS, and LSV techniques. The XRD pattern (JCPDS-41-1471) confirmed that the product was cubic metallic cobalt pyrite (CoS₂). UV-DRS revealed a narrow band gap of about 0.8 eV, consistent with its metallic nature. FE-SEM images showed that the material formed hollow microspheres composed of nanosheets with internal voids. The synthesized material functions as an efficient electrocatalyst for the hydrogen evolution reaction (HER), as demonstrated through electrochemical evaluations using CV, LSV, and EIS techniques. CoS₂ exhibits remarkable electrochemical behaviour, attributed to its metallic conductivity and abundant active sites. It delivers encouraging results, including low overpotential values and Tafel slopes, which emphasise its rapid and effective HER kinetics.

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O68. Development of Standard Cosmetic Formulations as Reference Prototypes for Future Eco-Friendly Bioformulations from Moroccan Biomass By-Products

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The cosmetic sector is currently facing major challenges due to increasing consumer demand for natural, sustainable, and non-toxic products, as well as growing environmental concerns regarding synthetic ingredients and their impact on human health. The widespread use of potentially irritating or allergenic compounds in conventional formulations remains a critical constraint for the development of safe and eco-friendly cosmetics. As part of a broader thesis aiming to valorize Moroccan biomass by-products in cosmetic bioformulations, this study focuses exclusively on the elaboration and characterization of standard cosmetic formulations without any biomass incorporation. These conventional formulations serve as reference prototypes for future comparisons with eco-friendly prototypes that will subsequently integrate bioactive ingredients derived from local biomass. The synthesized prototypes were prepared following classical protocols adapted to each formulation type. The resulting products were subjected to comprehensive quality controls, including pH measurement, viscosity assessment, centrifugation stability, organoleptic evaluation, contact angle measurement, Fourier-transform infrared (FTIR) spectroscopy, and free alkalinity testing. The results confirmed the formation of stable, homogeneous, and suitable cosmetic bases with appropriate physicochemical properties. This foundational work establishes reproducible protocols and provides essential reference data. In future studies, the performance and safety of novel, biomass-enriched ecological cosmetic prototypes will be evaluated against these reference prototypes on cutaneous epithelial tissue.

O69. Optimization of cobalt-free mixed ionic-electronic conducting electrodes for solid oxide cells

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The development of high-performance oxygen electrodes for solid oxide cells (SOCs) remains strongly dependent on cobalt- and strontium-based materials, which present critical drawbacks such as environmental impact, associated health problems, and long-term instability due to surface segregation and degradation phenomena. These limitations have driven the search for alternative cobalt-free mixed ionic-electronic conductors (MIECs). In this context, lanthanum nickelates have emerged as promising candidates. However, despite their compositional advantages, they are limited by oxygen diffusion, which follows a preferential path at the surface. In this work, the electrochemical performance of $\text{La}_2\text{NiO}_{4+\delta}$ (L2N1) and $\text{La}_4\text{Ni}_3\text{O}_{10-\delta}$ (L4N3) was investigated, focusing on the effect of praseodymium oxide (PrO_x) infiltration on oxygen reaction kinetics [1]. The materials were applied as symmetrical electrodes on $\text{La}_{0.8}\text{Sr}_{0.2}\text{Ga}_{0.8}\text{Mg}_{0.2}\text{O}_{3-\delta}$ (LSGM) electrolytes. Structural analysis confirmed phase purity and chemical compatibility, while microstructural characterization revealed porous and well-adhered electrode layers. Electrochemical impedance spectroscopy (EIS) measurements performed between 600 and 800 °C under varying oxygen partial pressures demonstrated that L2N1 exhibits superior performance compared to L4N3, attributed to its higher ambipolar conductivity driven by enhanced oxygen-ion diffusion. PrO_x infiltration led to a significant reduction in polarization resistance (R_{pol}), decreasing by approximately 7-fold for L2N1 and 17-fold for L4N3 at 700 °C. These enhancements are attributed to the catalytic role of PrO_x , which promotes oxygen dissociation and accelerates charge transfer at the electrode surface. Among the studied materials, the L2N1+ PrO_x electrode showed the best overall performance, reaching R_{pol} values as low as $\sim 0.2 \, \Omega \, \text{cm}^2$ at 800 °C. These findings highlight the potential of PrO_x -infiltrated RP nickelates as efficient and stable oxygen electrodes for SOC applications.

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O70. What catalysts can enable hydrocarbon-fuelled protonic ceramic cells?

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Protonic ceramic cells (PCCs) operating on hydrocarbons offer a promising route for the efficient utilisation of carbon-containing fuels, including greenhouse gas-rich streams, yet conventional Ni-based anodes suffer from coking and redox instability. Transition metal (oxy)carbides emerge as potential alternatives due to their structural stability and carbon tolerance; however, their behaviour in realistic fuel environments remains poorly understood. In this work, several (oxy)carbides are evaluated as fuel electrodes, with particular focus on molybdenum (oxy)carbide ($\text{Mo}_2\text{C}_x\text{O}_y$) combined with $\text{BaCe}_{0.9}\text{Y}_{0.1}\text{O}_{3-\delta}$ (BCY) [1]. Among the compositions studied, only $\text{Mo}_2\text{C}_x\text{O}_y$ demonstrates chemical compatibility with the BCY electrolyte, together with phase stability in methane and hydrogen.

Electrochemical testing at 800 °C in humidified methane reveals an ~82 % decrease in polarisation resistance over one week, indicating a self-activation behaviour. This improvement arises from dynamic recarburisation, which increases the C/O ratio in the anionic sublattice, promotes lattice expansion, and enhances catalytic and electronic properties.

A key limitation of transition metal (oxy)carbides lies in their instability in biogas environments: exposure to CO_2 leads to oxidation, with rapid kinetics at high temperatures. Although a stability window exists at lower temperatures (~600 °C), thermodynamic analysis indicates that methane reforming remains limited under these conditions, which is reflected in the decrease of the open-circuit voltage from ~0.8 V at 800 °C to ~0.5 V at 700 °C.

Overall, these results identify molybdenum (oxy)carbide as a promising catalyst for hydrocarbon-fuelled PCCs, owing to its self-activation behaviour and carbon tolerance, and establish a structure–property–function relationship governed by the anionic composition of the (oxy)carbide, while highlighting critical challenges for their implementation in biogas-fuelled systems.

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O71. Proton therapy assisted by palladium nanospheres (Pd Sph) and palladium nanocubes (Pd Cub) – *in vitro* studies

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Palladium nanoparticles (Pd NPs) have recently emerged as a promising alternative to gold nanoparticles (Au NPs) in biomedical applications, particularly as radiosensitizers. In this study, we investigate the potential of shape-controlled Pd NPs as radiosensitizers in proton radiotherapy [1-4]. Two types of Pd NPs – spherical (Pd Sph) and cubic (Pd Cub) – were synthesized using comparable reaction conditions to isolate the effect of shape while maintaining similar size and surface chemistry.

To improve biocompatibility and cellular uptake, the Pd NPs were functionalized with thiolated glucose, taking advantage of the enhanced glucose metabolism in cancer cells (Warburg effect) [5-6]. Successful functionalization was confirmed by FTIR spectroscopy. The cytotoxicity and radiosensitizing potential were evaluated using MTS assays, allowing the determination of critical concentrations that do not significantly affect cell viability. Glucose-modified Pd NPs demonstrated reduced cytotoxicity and enabled the use of higher concentrations, enhancing their potential as radiosensitizers.

Advanced holotomographic microscopy was applied to study Pd NPs – cells interactions in a label-free and real-time manner. This technique enabled three-dimensional visualization of cells based on refractive index distribution, allowing the assessment of Pd NPs uptake dynamics, intracellular localization and morphological changes. The results indicated increased cellular uptake for glucose-modified Pd NPs compared to non-modified systems. Interestingly, Pd Cub exhibited slightly higher uptake than Pd Sph; however, no statistically significant differences in radiosensitization were observed between the two shapes.

Overall, this work demonstrates that properly designed Pd NPs can act as effective and potentially cost-efficient radiosensitizers in proton therapy. The combination of surface functionalization and advanced imaging techniques provides valuable insight into NPs-cells interactions and opens new perspectives for the development of targeted and multimodal nanotherapeutic systems.

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O72. Graphene-Based Ternary Nanocomposites for Water Purification Applications

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Abstract: Water pollution caused by industrialization and urbanization has become a major global challenge, necessitating the development of advanced and efficient treatment technologies. Graphene oxide (GO)-based ternary nanocomposites have emerged as promising materials for water purification due to their unique physicochemical properties and multifunctional capabilities. This review provides a comprehensive overview of the synthesis, properties, performance enhancement, and environmental applications of GO-based ternary nanocomposites. GO, with its high surface area, abundant oxygen-containing functional groups, and excellent dispersibility, serves as an ideal platform for constructing hybrid nanocomposites. The incorporation of metal or metal oxide components along with a third functional material enables synergistic interactions that enhance adsorption capacity, photocatalytic efficiency, and antimicrobial activity. Various synthesis methods, including Hummers' method for GO preparation and hydrothermal, sol-gel, co-precipitation, and green synthesis techniques for nanocomposite fabrication, are discussed. The mechanisms of water purification involve adsorption, photocatalysis, and antibacterial action, enabling effective removal of heavy metals, dyes, organic pollutants, and pathogens. Performance enhancement strategies such as band gap tuning, heterojunction formation, and surface modification further improve efficiency and stability. Additionally, the review highlights the wide range of environmental applications of these nanocomposites in wastewater treatment and water disinfection. However, challenges related to toxicity, environmental impact, cost, scalability, and material recovery remain significant barriers to practical implementation. Future research should focus on sustainable synthesis, improved recyclability, and comprehensive risk assessment to ensure safe and large-scale application of these materials.

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O73. Phase Stability of Ruddlesden–Popper Ba_2SnO_4 under reducing atmosphere to Proton Ceramic Cells

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Proton ceramic fuel cells (PCFCs) have gained increasing interest as efficient and cost-effective energy conversion devices, offering fuel flexibility and strong potential for electrical power generation [1]. The Ruddlesden–Popper oxide $\text{Ba}_2\text{SnO}_{4-\delta}$ has attracted increasing attention for energy-related applications due to its layered structure and redox-active Sn cations. However, its phase stability under fuel-processing conditions relevant to proton ceramic devices remains insufficiently understood [2].

In this work, the structural evolution, defect chemistry, and phase stability of $\text{Ba}_2\text{SnO}_{4-\delta}$ were systematically investigated under reducing atmospheres using powder X-ray diffraction, bond valence analysis, and thermodynamic calculations. Under nominally dry H_2 , $\text{Ba}_2\text{SnO}_{4-\delta}$ retains its tetragonal Ruddlesden–Popper structure up to 700 °C through a topotactic reduction mechanism involving significant oxygen vacancy formation and partial reduction of Sn^{4+} to Sn^{2+} . The process is accompanied by anisotropic structural relaxation, including shortening of apical Sn–O bonds and contraction along the c-axis, while bond valence analysis reveals a progressive decrease in the average Sn oxidation state. Oxygen vacancies preferentially form at equatorial sites, whereas apical oxygen occupancy remains largely unchanged. Tolerance factor analysis rationalizes the observed stability window, with moderate reduction preserving structural integrity and extensive reduction leading to structural collapse at higher temperatures.

In contrast, wet H_2 induces partial decomposition at 600 °C, while exposure to CO_2 results in complete decomposition into BaSnO_3 and BaCO_3 due to carbonation of BaO layers. Conversely, the structure remains comparatively stable in dry CH_4 . These findings demonstrate that phase stability is strongly governed by gas composition and the chemical reactivity of BaO rock-salt layers, highlighting intrinsic limitations and guiding strategies for improving the durability of layered barium stannates in proton ceramic applications.

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O74. An Efficient and Sustainable Metal-Free Synthesis of Highly Substituted Piperidines Derivatives under Ultrasound Irradiation

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Piperidine derivatives constitute a privileged class of Nitrogen-containing heterocycles that are widely present in natural products and play an important role in pharmaceutical drug discovery and development. Due to their significant importance, the development of efficient, sustainable piperidine motifs remains highly desirable. Herein, we report a green and efficient ammonium chloride-catalysed one-pot multicomponent strategy for the synthesis of highly substituted piperidine derivatives via the reaction of aromatic aldehyde, aromatic amines, and β -ketoester under ultrasound irradiation. The developed methodology offers several significant advantages, including the use of easily available, inexpensive, and eco-friendly catalysts, operational simplicity, short reaction times, high efficiency, and a straightforward workup procedure that typically involves simple filtration. Overall, this protocol provides a practical, sustainable, and metal-free approach for the efficient synthesis of functionalized piperidine derivatives.

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O75. Influence of Cu:Ag Composition on Ionic Release and Longevity of Wearable Dry Electrodes

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Functional metallic thin films for wearable biopotential electrodes have attracted increasing interest due to their potential to combine conductivity, durability, and biocompatibility in long-term health-monitoring applications. Among these systems, dry electrodes based on Ag and Cu coatings offer promising electrochemical and antimicrobial properties while enabling integration into low-cost wearable platforms [1, 2]. In this work, Ag and Cu thin films were deposited onto stereolithography-printed poly(lactic acid) resin substrates to prepare dry biopotential electrodes for wearable sensing applications. Two Cu:Ag compositions (50:50 % and 10:90 %) were investigated in order to evaluate the influence of metallic composition on ionic release behaviour and stability over time. The simultaneous quantification of released Ag and Cu ions was accomplished by anodic stripping voltammetry (ASV), enabling sensitive monitoring of ion release kinetics and degradation processes [3].

The results demonstrate distinct temporal release profiles depending on film composition, indicating the influence of metallic composition on electrode stability and ionic release behaviour over time. These findings contribute to the development of functional metallic interfaces for wearable bioelectronic systems and provide insights into the design of durable dry electrodes for continuous biopotential monitoring applications.

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O76. Incorporation of graphene oxide in concrete: from car batteries to reinforced construction materials

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The growing usage of lithium-ion batteries has intensified the demand for recycling strategies for its constituents. Graphite plays an essential role as the anode material in this type of batteries and has been classified as a critical strategic raw material by the European Union [1]. Graphene oxide (GO) can be synthesized from graphite and is a material of growing relevance in advanced materials science. Currently, graphite is being generated as a component of the black mass, which also comprehends metallic elements, produced during the recycling of end-of-life batteries by b.again (dstgroup). Its effective valorization for other applications presents an important opportunity within the framework of circular economy and sustainable materials development.

GO can be added to concrete mixtures as a colloidal suspension. The result is an enhancement of the concrete's mechanical properties, with a more compacted structure and improved resistance to compressive and flexural strength. Furthermore, it presents an opportunity for the reduction in material usage and costs in construction.

In this work, GO was synthesized by the improved Hummers method from purified recycled graphite supplied by b.gain and its quality was validated by comparison with other GO samples acquired from a commercial supplier and synthesized by the same method but from a commercially acquired 100 µm graphite and pencil graphite [2]. The resulting product materials were characterized by attenuated total reflectance - Fourier-transform infrared spectroscopy (ATR-FTIR), X-ray fluorescence spectroscopy (XRF), ultraviolet-visible spectroscopy (UV-Vis) and Raman spectroscopy. Furthermore, the applicability of GO as an additive to enhance the performance of concrete mixtures will be evaluated through compressive and flexural tests on concrete samples without GO and with GO synthesized from purified recycled graphite and acquired from a commercial supplier.

This study highlights an effective pathway to produce high-quality GO and the valorization of graphite from spent lithium-ion batteries for the development of smart construction materials.

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O77. Tailoring the Microstructure and Electrical Properties of Ti-Au Thin Films via Glancing Angle Deposition for Dry Electrode Applications

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Abstract

This study investigates the optimization of titanium-gold (Ti-Au) thin films developed by Glancing Angle Deposition (GLAD) to develop dry electrodes for electromyography (EMG). By changing the growth geometry during magnetron sputtering, a physical vapor deposition process, distinct microstructures, including conventional, inclined, and zig-zag geometries, were developed with varying Au compositions and deposition angles. The correlation between the microstructural geometry and subsequent electrical properties was systematically evaluated. The results demonstrate that while increasing Au content effectively reduces electrical resistivity, deposition angles exceeding 60° introduce significant microstructural effects that increase the electrical resistivity of the film. Crucially, these thin films' architectures allow for a highly adjustable balance between electrical conductivity and mechanical flexibility. This work highlights how composition and growth geometry serve as fundamental design parameters for optimizing thin films, establishing a foundation for forthcoming investigations into their mechanical behavior and biocompatibility.

Introduction

The increasing prevalence of age-related motor disabilities has increased the demand for innovative healthcare solutions [1]. Electromyography (EMG), which records muscle activity, is essential for detecting neuromuscular disorders and enabling personalized treatment. Although Ag/AgCl wet electrodes are widely used, their dependence on conductive gel can lead to discomfort and hinder long-term use. In contrast, dry electrodes provide a more comfortable and practical solution for prolonged monitoring [2]. This study aims to investigate the use of titanium-gold (Ti-Au) thin films as potential dry electrodes, due to their biocompatibility and promising flexibility and electrical conduction. The films were deposited by magnetron sputtering using the glancing angle deposition (GLAD) technique, and the effects of composition and growth geometry on their electrical performance were systematically evaluated.

- Method

Ti-Au thin films were deposited on silicon and glass substrates using direct current magnetron sputtering by GLAD. The films were grown in different geometries: conventional, inclined, and zigzag, using deposition angles ranging from 0° to 90° and prepared in different chemical compositions (Au/Ti ratio ranging from 0 to 0.80). The electrical resistivity of the thin films was measured using the four-point probe method, and their crystalline structure and microstructure were characterized by X-ray diffraction and transmission electron microscopy, respectively.

- Results

For the low tested range of Au/Ti ratios, increasing the gold content seems to result in a tendency toward reduced resistivity relative to the Ti pure thin films, regardless of the deposition angle. Regarding the effect of growth geometry, the electrical resistivity of the Ti-

Au thin films tends to increase for deposition angles above 60° . Despite this trend, the films continue to exhibit high electrical conductivity while enabling tailored mechanical flexibility.

- Discussion

The film's microstructure was found to significantly influence the electrical properties of Ti-Au thin films deposited at 70° or higher, suggesting that microstructural effects, together with chemical composition, play a crucial role in the overall electrical resistivity of the films.

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O78. Nanostructured Flexible Dry-Electrodes for Personalized and Preventive Digital Healthcare

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In a context of continuous progress in healthcare, digital medicine has become central to ensuring effective, accessible, and preventive care. Within this framework, wearable and remote monitoring technologies play a key role in enabling continuous physiological assessment outside traditional clinical settings. Among these, dry electrodes have emerged as enabling components for modern digital health systems, due to their ease of integration into wearable platforms and suitability for long-term monitoring [1]. The innovative evolution of dry electrodes based on thin films extends their applicability to digital medicine, particularly in the development of wearable and connected systems for remote monitoring and therapeutic intervention. These technologies facilitate the implementation of closed-loop biofeedback architectures, applicable in both clinical and home environments, where real-time sensing and actuation can be combined to support adaptive interventions. Such systems enable personalized stimulation and feedback strategies, contributing to more targeted and responsive therapeutic approaches, particularly in neuro-rehabilitation contexts.

In this framework, the present work focuses on the development of integrated platforms that combine electroencephalography (EEG), electromyography (EMG), electrocardiography (ECG), and functional electrical stimulation (FES), with the objective of enabling closed-loop neuromodulation strategies. Biocompatible electrodes based on nanostructured Ti-based thin films are prepared by magnetron sputtering, with tailored electromechanical and electrochemical properties, exploring different compositions, structures and morphologies. These nanoscale-designed thin films are deposited on biodegradable and flexible polymeric materials, enabling sensing and stimulation [1-5]. When combined with machine learning algorithms, the resulting systems support multimodal physiological monitoring and adaptive stimulation strategies, advancing the development of intelligent, patient-specific digital therapeutic platforms [3,5].

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O79. Investigation of the influence of titanium dioxide (TiO₂) on Carboxymethyl Cellulose (CMC) based hydrogels

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Hydrogels are materials composed of a three-dimensional network of polymer chains. They are capable of absorbing relatively large amounts of fluids [1]. Due to their biocompatibility and their properties, hydrogels are used in many applications such as biomedical engineering and materials science [2]. Carboxymethyl cellulose (CMC) is a water-soluble cellulose derivative [3]. Commonly used as a thickening agent, CMC is a suitable component for hydrogels formation. The incorporation of titanium dioxide (TiO₂), can modify the structure of hydrogel and physicochemical properties. Thus, the influence of titanium dioxide incorporation on the CMC-based hydrogel was studied using different analytical methods. The influence of titanium dioxide incorporation on the hydrogel was studied using different analytical methods. UV–visible spectroscopy was used to evaluate the photodegradation of methylene blue in aqueous solution under UV irradiation. Zeta potential measurements and particle size distribution analyses were performed to evaluate the stability of the hydrogels. Fourier-transform infrared spectroscopy (FTIR) was also used to determine any changes in chemical bonding occurred, while morphological properties were analyzed using scanning electron microscopy (SEM). Finally, swelling tests were carried out on the hydrogels to determine their water absorption capacity.

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O80. Preparation and Characterization of P-123 Stabilized Functionalized Multi-Walled Carbon Nanotube Particles

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Carbon nanotubes (CNT) are widely used nanomaterials due to their remarkable electrical, thermal, and mechanical properties. However, their strong tendency to aggregate in aqueous media limits their practical applications. In this study, functionalized multi-walled carbon nanotubes (MWCNT-COOH) were dispersed and stabilized using Pluronic P-123 polymer under low-temperature conditions.[1]

A cold aqueous P-123 stock solution was prepared in an ice bath at approximately 4°C to prevent premature gel formation and to obtain a homogeneous dispersion medium. Functionalized MWCNT-COOH particles were added to the prepared P-123 solution and homogenized using sonication for 15 minutes. The obtained dispersions were characterized using UV-Vis spectroscopy, Dynamic Light Scattering (DLS), Zeta Potential analysis, and FTIR-ATR spectroscopy.

UV-Vis measurements confirmed the successful dispersion of carbon nanotubes in aqueous media, while particle size and zeta potential analyses demonstrated improved colloidal stability of the system. FTIR spectra confirmed the presence of characteristic absorption bands of P-123. Due to overlap of absorption bands and the weak infrared response of carbon nanotubes, CNT-related signals were not clearly distinguished. However, Raman analysis supported the presence of functionalized carbon nanotubes in the system [2].

The obtained results demonstrate that Pluronic P-123 is an effective stabilizing agent for functionalized carbon nanotube dispersions and may provide potential applications in nanotechnology, hydrogel systems, biomedical materials, and advanced composite studies.

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O81. Photocatalytic Degradation of Methylene Blue Using TiO₂/Carboxymethyl Cellulose Hydrogel Films

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Synthetic dyes released from industrial processes, particularly textile manufacturing, constitute a major environmental concern due to their persistence and toxicity in aquatic environments [1]. Semiconductor-based photocatalysis has emerged as an effective approach for the degradation of organic pollutants, with TiO₂ being one of the most widely used photocatalysts because of its high stability, low cost, and excellent photocatalytic activity under UV irradiation [2]. However, the recovery of TiO₂ nanoparticles from treated water remains a significant challenge.

In this study, anatase-phase TiO₂ nanoparticles were synthesized via a hydrothermal method and incorporated into crosslinked carboxymethyl cellulose (CMC) hydrogels. The hydrogel matrix was employed to facilitate catalyst recovery while enhancing dye adsorption through its hydrophilic three-dimensional network structure [3]. The photocatalytic performance of the prepared TiO₂/CMC composite hydrogels was evaluated through the degradation of methylene blue under UV light. In addition, FTIR spectroscopy, contact angle measurements, and swelling capacity analyses were performed to investigate the structural and surface properties of the synthesized materials.

The developed TiO₂/CMC hydrogels combine adsorption and photocatalytic degradation within a single recoverable material, highlighting their potential for sustainable wastewater treatment applications [4].

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O82. Tailoring Spin Textures in Two-Dimensional Chromium Nitride via Half-Halogenation

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We study the magnetic behavior of half-halogenated two-dimensional CrN (F–CrN and Cl–CrN) using density functional theory combined with effective spin modeling. Breaking inversion symmetry through halogenation generates finite Dzyaloshinskii–Moriya interaction (DMI), which drives the formation of chiral spin textures. Our calculations indicate that Cl–CrN supports stable Néel-type skyrmions at moderate magnetic fields (~50 T), within reach of present high-field experimental setups. In comparison, F–CrN favors antiskyrmion configurations but only under much stronger fields (~275 T), reflecting its enhanced DMI strength. Such extreme fields remain challenging but are accessible in pulsed-field experiments. These results highlight halogen substitution as an efficient mechanism to control DMI strength and tailor distinct topological spin states in CrN, making these systems promising candidates for future spintronic technologies.

Poster presentations

P1. Surface effects on mode-I crack tip fields: A finite element simulations

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In this paper, we investigate how surface effects (surface elasticity and surface tension) influence the near-tip stress and deformation fields of a mode-I crack in an elastic solid, particularly at the nanoscale where the crack tip curvature radius is on the order of nanometers.

The study uses the finite element method developed by He [1-2] which incorporates the theory of Gurtin and Murdoch's surface elasticity [3] to analyze these effects.

As a result, we show that:

- Surface effects are significant when the curvature radius of the crack tip is on the order of nanometers.
- Surface effects modify local stress distributions, particularly the positions and magnitudes of maximum stresses around the crack tip.

We can therefore conclude that surface effects impact local stress fields around cracks at the nanoscale.

This work contributes to the understanding of fracture phenomena at the nanoscale and highlights the importance of surface effects in modern materials.

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P2. Tuning Crystal Facets of BiVO₄ for Enhanced Charge Separation

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Bismuth vanadate (BiVO₄) has emerged as a promising and stable visible-light-responsive semiconductor for a wide range of solar-driven applications such as photocatalysis, photoelectrochemical energy conversion, and environmental remediation and etc. Despite these advantages, its overall performance is often limited by inefficient charge separation and transport, which restrict the utilization of photogenerated charge carriers [1].

Recent studies have demonstrated that the photoactivity of BiVO₄ is strongly influenced by particle morphology and, more importantly, by the nature of exposed crystal facets. Different facets of BiVO₄ possess distinct atomic arrangements, surface energies, and electronic structures, leading to facet-dependent charge-carrier migration, surface charge distribution, and adsorption behavior. It has been reported that photogenerated electrons and holes preferentially migrate to different facets, enabling spatial charge separation within a single particle. Some facets (e.g., {010}) have often been associated with electron-rich behavior, while different facet like {110} tend to favor hole accumulation, resulting in enhanced charge separation efficiency. Therefore, facet engineering can significantly affect surface reactivity, selectivity, and stability across various photocatalytic and photoelectrochemical processes, including selective reduction/oxidation reactions. Recent studies have shown that the photoactivity of BiVO₄ is strongly influenced by particle morphology and the nature of exposed crystal facets, which govern charge-carrier transport pathways and surface reaction sites [2-3].

In this work, BiVO₄ crystals with distinct dominant facets were synthesized via a hydrothermal method by systematically adjusting the solution pH, enabling controlled modulation of crystal morphology and facet exposure. The phase composition and crystallinity of the synthesized materials were confirmed by X-ray diffraction (XRD), while scanning electron microscopy and particle size distribution analysis revealed significant differences in particle size and morphology among the samples. The surface charge properties were further investigated by determining the point of zero charge, providing insight into facet-dependent surface chemistry and interfacial interactions.

Facet-specific charge separation behavior was examined using selective Ag photodeposition to identify preferential photogenerated electron accumulation sites. The photoelectrochemical performance of the BiVO₄ samples was evaluated by linear sweep voltammetry, while charge-transfer processes and recombination dynamics were analyzed using electrochemical impedance spectroscopy under both dark and illuminated conditions. The results demonstrate a correlation between morphology, exposed crystal facets, surface charge characteristics, charge separation efficiency, and photocurrent response and charge transport properties.

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P3. The Nanoscience Dalmatian: Metal Decorated Titanium Dioxide Nanoparticles via Spark Ablation

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It is difficult to overestimate the importance of titania (TiO₂) for material science applications. This unique material is studied due to its photoactivity and semiconductor properties. Moreover, the low cost of TiO₂ contributes to its attractiveness. For further enhancement of electronic and optical properties of TiO₂, a lot of research was conducted on semiconductor modification with transition metals.¹

Our research is focusing on the optimization of TiO₂ coating with metals *via* Spark Ablation for CO₂ photoreduction. Despite a wide range of 'wet' synthesis procedures, typically they are time consuming and often require environmentally unfriendly metal precursors. This is not the case for the generation of metal nanoparticles *via* Spark Ablation which is a precursor-less method.²

Our main goal was to generate a system that has a real-life application. Therefore, Au, Pt, Cu and Ni were chosen as metals that are commonly used for heterogeneous CO₂ reduction. Despite being close neighbours in the Periodic table, each metal revealed a unique TiO₂ decoration behaviour.

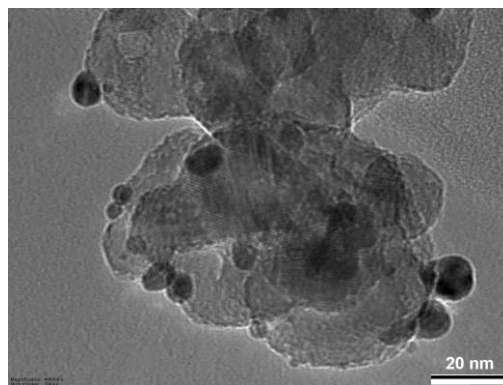


Figure 1 – TEM image of Au nanoparticles coated TiO₂.

Au forms single nanoparticles with distinct spherical shape that can be clearly detected on TiO₂ surface (Figure 1). In case of Pt and Ni, nanoparticles have a strong tendency to coagulate to fractal-like agglomerates that attach to TiO₂. Cu demonstrates a unique behaviour and coats the TiO₂ surface with a veil-like layer of nanoparticles.³

The obtained systems revealed promising CO₂ into methane photocatalytic conversion.

For the characterization of TiO₂ coating with nanoparticles several complementary techniques were used: Scanning Mobility Particle Sizer (SMPS), electron microscopy (SEM, TEM) and energy dispersive X-ray spectroscopy (EDX) as well as Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES).

Titania is a key material for numerous applications like heterogeneous catalysis, water splitting and many more. A simple and efficient TiO₂ decoration procedure allows accessing a broad variety of applications with improved performances.



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P4. Investigation of physical properties of new Silicon Telluride compounds from First-Principles Calculations

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Silicon telluride (Si₂Te₃) is a new low –dimensional 2D material recently synthesized. First principles calculation is used to predict structural properties of Si₂Te₃ at the trigonal structure. Elastic constants confirm the mechanic stability of silicon telluride. Various mechanical parameters, including (Young's E, bulk B, shear G, Pugh's) modulus, Poisson's ratio and anisotropy factors are also determined. Results of electronic Band structure show that the Si₂Te₃ is an semiconductor with bandgap equal to 1.52 eV. Furthermore, we determined frequencies of vibrational phonon using phonopy programs. Results show that all frequency are positive confirming stability of this material.

P5. Overview of binary noble metal-rare earth compounds

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Alloys based on rare earth(Re)- noble metal(Nm) are of great importance in the field of electronics and electromagnetics due to their specific properties linked to the presence of electrons. In this work presenting us with a statistical study on the presence of the defined compounds in the Mn-RE phase diagrams at different stoichiometry.

We found that all diagrams based on Au-Re and Cu-Re exhibit equiatomic compounds.

A Comparison of melting temperature according to atomic number of rare earth element is presented.

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P6. Designing Materials with Optoelectronic and Photovoltaic Properties as Potential Dopant-free Hole Transport Materials for Advanced PSCs

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The development of efficient, dopant-free hole-transport materials (HTMs) remains a key challenge for manufacturing stable and scalable perovskite solar cells. Here, we design and computationally explore photovoltaic potential of a series of five dithienylethene derivatives (DTE1–DTE5) that constructed by end-capping a NaDTE core with thiophene spacers and electron-accepting terminal groups as suitable potential dopant free hole transport materials (HTMs). Using DFT and TD-DFT calculations (B3LYP/6-31G(d,p), IEFPCM-THF), we reveal how subtle electronic modulation drastically tuned the molecular frontier levels, optical activity, and charge transport behavior. The designed molecules exhibited narrowed HOMO–LUMO gaps (2.21–2.69 eV) relative to reference NaDTE (4.09 eV), accompanied by pronounced red-shifts in optical absorption ($\lambda_{\text{max}} = 514\text{--}633\text{ nm}$) and enhanced oscillator strengths ($\text{LHE} > 0.93$). Charge-transport analyses show reduced reorganization energies ($\lambda_{\text{e}} \approx 0.12\text{--}0.21\text{ eV}$) and high hole-transfer integrals (th up to 0.252 eV), indicating efficient carrier mobilities in these designed molecules. Solvent-phase dipole moments reached 15.6 D (DTE2), further supporting superior solubility and interfacial compatibility. Theoretical photovoltaic metrics suggest open-circuit voltages in the range of 1.44–1.69 V and comparative power conversion efficiencies of 32–38%, demonstrating high potential of these materials as dopant-free HTMs for advanced PSC photovoltaics. Among the designed ones, DTE2 and DTE5 emerged as the most balanced candidates, based on their strong absorption, favourable reduced band gaps, robust charge transport and better photovoltaic properties.

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P7. Chiral and Entropic Interactions in Self-Assembly of Cellulose Nanocrystals (SCNCs) into Optically Active liquid crystals

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Nanocellulose is a bio-based, non-toxic, degradable source used for preparation of nano-structured functional coatings. Cellulose nanocrystals (CNCs) can be derived from agricultural and industrial waste via mild-acid-hydrolysis. When the sulfuric-acid hydrolysed CNCs are dispersed in aqueous solutions they self-assemble into a liquid crystalline phase (LC), that can be used for preparation of large area, micron-thick chiral nematic films that selectively reflect circularly polarized light at a wavelength that is determined by organization of the nanoparticles.

We experimentally investigated the effect of a chiral environment and the effect of a non-adsorbing natural hydrocolloid (Gum Arabic) on the self-assembly of CNCs.

Our observations reveal 1) Disruption and modification CNCs assembly in solutions of enantiomerically pure D-alanine. In this system the effect is specific to D-alanine and cannot be attributed to the adsorption of alanine molecules (neither D- nor L-alanine) onto the CNC particles [1] 2) A non-adsorbing GA hydrocolloids affects the phase behavior and organization of suspended CNCs [2]. We observe that the inter-particle distance and the chiral pitch of the N* phase are determined by the concentration of GA (for a given CNCs concentration). The resulting mesophases were characterized *via* transmission electron microscopy at cryogenic temperatures (cryo-TEM), small-angle X-ray scattering (SAXS), and polarized optical microscopy (POM). Our findings indicate that GA can be used to tune the phase diagram and optical properties of SCNC suspensions, and overcome kinetic barriers that lead to gelation or kinetic arrest.

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[2] D. Attia, Y. Levi-Kalishman, R.Bitton and R. Yerushalmi-Rozen *Nanoscale Advances* **7**, 1617-1626 (2025).

P8. Tolerance synthesis in mechanical assemblies using Monte Carlo simulation

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In many industries, cost and manufacturing accuracy are closely related. The tolerances used have a big influence on product quality and cost.

Sophisticated materials and procedures are needed to achieve tight tolerances, which raises costs. Wide tolerances, on the other hand, are more cost-effective since they enable production with a lower material investment. Thus, selecting tolerances is one of the most important phases in design optimization.

This work proposes a statistical approach to redefine geometric tolerances based on the Jacobian Torsor model. The Jacobian Torsor model is used to characterize the functional relationship between the assembly's functional requirements and the functional elements that make it up.

Monte Carlo simulation is then used to determine statistical bounds.

Critical tolerances are redefined to satisfy the given functional need by redistributing tolerances according to the proportional contribution of each functional element to the overall requirement. A practical case study, using parts produced by additive manufacturing, is used to demonstrate the efficacy of the suggested method.

P9. Magnetron-sputtered AZO thin films on 3D-printed substrates for sEMG and SmO₂ sensing

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Chronic back pain in adolescents and young adults has become a pressing concern in modern society. The increasing use of smartphones, laptops, and sedentary study habits has led many young adults to spend more than eight hours per day in forward-flexed postures. Surveys suggest that non-specific neck and back pain now appear before the age of sixteen in a significant proportion of the population, and chronic postural deviation during this developmental stage may set the trajectory for musculoskeletal dysfunction well into adulthood.

Conventional braces and static support systems often show poor long-term compliance due to movement restriction and the absence of active feedback. Therefore, wearable devices capable of active posture correction may provide a more effective solution for this problem. Surface electromyography (sEMG) can continuously monitor the electrical activity of muscles, distinguishing in near real-time between deliberate exertion and the low-grade, sustained muscle tension associated with poor postural loading. When a predefined threshold is exceeded, the signal can be routed to electroactive polymer actuators integrated into wearable systems, which selectively contract or stiffen to guide the user back toward a neutral posture. Sustained muscular contraction, even at low intensities, can progressively impair local tissue oxygenation, accelerating the onset of fatigue and consequently promoting postural degradation. Skeletal muscle oxygen saturation (SmO₂), measured non-invasively through near-infrared spectroscopy (NIRS), can provide an additional monitoring layer within the posture correction process, enabling modulation of correction intensity or prompting the user to rest.

Combining sEMG and SmO₂ sensing in a single wearable platform is not straightforward. The main challenge comes from the optical requirements of SmO₂, as NIR light must penetrate the underlying tissue and return to the detector. This means the electrode cannot be composed of opaque conductive metals that dominate biosignal acquisition. Transparent conducting thin films offer a potential solution. When deposited over transparent polymeric substrates, these materials can maintain the electrical conductivity required for sEMG acquisition while remaining sufficiently transparent within the relevant spectral window to support optical oximetry. This dual-function architecture reduces the number of electrodes required on the wearable platform, simplifies garment integration, and may improve signal quality by enabling spatial co-registration of electrical and optical measurements from the same anatomical location.

In this work, aluminum-doped zinc oxide (AZO) thin films were deposited on 3D-printed substrates by magnetron sputtering, a physical vapor deposition (PVD) technique, aiming to develop transparent electrodes capable of simultaneously providing sEMG and SmO₂ monitoring.

P10. Deformations in nanocomposites of multiwalled carbon nanotubes and polymers, SiO₂

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Deformations in radiation, structural functionalized nanocomposites of multiwalled carbon nanotubes and polymers [1], SiO₂ is represented in Figure 1.

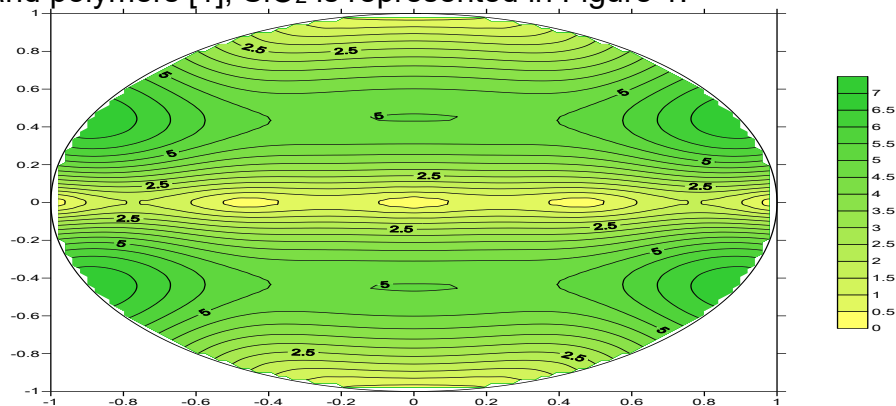


Figure 1 - The stereoprojection of polarization angle - deviation of the vector of elastic displacements $\vec{U}$ from the direction of the wave normal $\vec{n}$ $\phi_p = (\vec{U}, \vec{n})$ SiO₂ (isolines - in degrees).

Conclusion

1. Shear modulus G , elastic modulus E , internal friction Q^{-1} , Poisson's coefficient μ of nanocomposite, SiO₂ depend on its anisotropy.

Acknowledgements. This work has been supported by Ministry of Education and Science of Ukraine: Grant of the Ministry of Education and Science of Ukraine for perspective development of a scientific direction "Mathematical sciences and natural sciences" at Taras Shevchenko National University of Kyiv.

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DOI: <https://doi.org/10.1007/s42452-025-07799-0>

P11. Vibration Characteristics of Double-Walled CNT@BNNT Nanotubes in Rotational Bearing Systems

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MECACOMP Laboratory, Department of Mechanical Engineering, Faculty of Technology, University of Tlemcen, Algeria

In this study, vibration behavior of a double-walled CNT@BNNT nanotube used as a rotational bearing are investigated. The combination of carbon nanotubes (CNTs) and boron nitride nanotubes (BNNTs) forms an excellent heterogeneous structure characterized by high thermal and compressive resistance, as well as superior piezoelectric and ferroelectric properties. These features make such composites highly promising for applications in rotation transmission nanosystems (RTS). In the proposed heterogeneous rotational bearing, the inner boron nitride nanotube (BNNT) serves as the rotor, while the outer carbon nanotube (CNT) functions as the stator. The Timoshenko beam theory is employed to model the double-walled nanotube, incorporating piezoelectric effects for the inner BNNT. Maxwell's electrostatic equations, together with the nonlocal strain gradient theory, are used to capture the piezoelectric behavior and size-dependent characteristics of the system. The interaction between the inner and outer nanotubes is modeled using van der Waals (vdW) forces. To determine the vibration response of the nanobearing system, the Galerkin method is applied. Finally, the effects of small-scale parameters, rotational speed, applied voltage, van der Waals forces, and boundary conditions are systematically investigated.



Company presentations



C1. Anton Paar

Anton Paar TriTec SA, Les Vernets 6, 2035 Corcelles-Cormondrèche (Neuchatel), Switzerland

Anton Paar TriTec

Anton Paar TriTec is the Mechanical Surface Characterization product line of the Anton Paar Group. It builds on more than 45 years of expertise in mechanical surface characterization. Its origins date back to the Swiss Watch Research Laboratory, later evolving into CSM Instruments SA in 1999 before joining the Anton Paar Group in 2013.



Anton Paar TriTec develops, manufactures, and supplies instruments for evaluating the mechanical properties of material surfaces. Its portfolio includes indentation testers, scratch testers, tribometers, and Calotest coating thickness instruments, enabling the evaluation of hardness, adhesion, wear, friction, and coating performance.



Recognized worldwide for its expertise in instrumented indentation, Anton Paar TriTec combines a broad force range from nano- to macro-indentation with advanced scratch testing and tribology solutions to deliver comprehensive mechanical surface characterization. This integrated approach helps researchers and manufacturers develop more durable materials, optimize coating performance, accelerate product development, and ensure reliable quality across industries including automotive, aerospace, electronics, medical devices, energy, and advanced manufacturing.

Anton Paar

Founded in 1922 and headquartered in Graz, Austria, Anton Paar is a global leader in precision measurement technology. The company develops and manufactures analytical instruments for research, industry, and quality control, serving customers in more than 110 countries.

Anton Paar's main technology areas include density and concentration measurement, rheology and viscometry, particle characterization, Raman spectroscopy, X-ray analysis (SAXS/XRD), and mechanical surface characterization through Anton Paar TriTec.

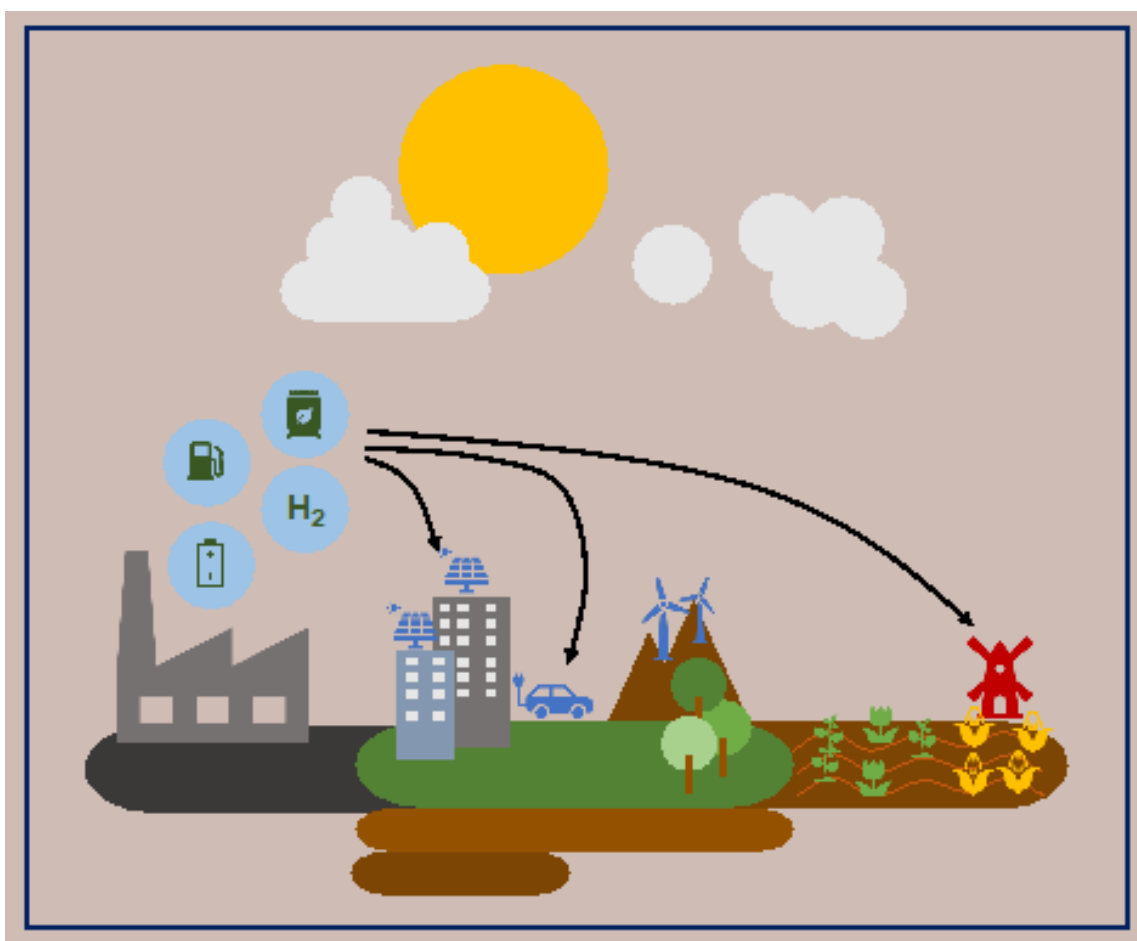
Today, Anton Paar employs over 4,000 people worldwide, operates 9 production sites, 35 sales subsidiaries, and collaborates with around 50 distribution partners. The company is owned by the Charitable Santner Foundation and invests approximately 16% of its annual turnover in research and development, supporting continuous innovation.

5th International Workshop on “Modern Trends in Energy Research”

IWMTER-2026

July 7, 2026, Aveiro, Portugal

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



Topics:

- ❖ Green Hydrogen: Production, Storage & Transport
- ❖ Fuel Cells/Electrolysers
- ❖ Electrochemical Synthesis of Green Fuels and Chemicals
- ❖ Batteries & Supercapacitors
- ❖ Power Engineering: Devices and solutions



- ❖ **Nanocatalysis & Electrocatalysts**
- ❖ **AI in Energy Research**

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. Francisco J. A. Loureiro (UA, Portugal)
Dr. Igor Bdikin (UA, Portugal)
Dr. Duncan Paul Fagg (UA, Portugal)

***No registration fee**

***This event is only in online mode**

Workshop Contact:

dpukazh@ua.pt

Deadline for abstract submission:

30th June 2026

Abstract format:

Any format in word (1 page)

Total Lectures: 10 (1 plenary + 1 keynote + 8 invited talks)

Time frame: (1*45 minutes) + (1*25 minutes) + 8 (20 minutes)

IWMTER 2026 Program

5th International Workshop on Modern Trends in Energy Research – IWMTER 2026

(In association with 8th International Conference on Nanomaterials Science and
Mechanical Engineering: ICNMSME-2026)

Centre for Mechanical Technology and Automation – TEMA, Department of Mechanical
Engineering, University of Aveiro, Portugal

7th July 2026, 9 h to 13.15 h

Session:1

Chair: Vanessa Graça

9.00 – 9.05	Workshop introduction and welcome Address D. Pukazhselvan (Convener IWMTER 2026)
9.05 – 9.50	Plenary Lecture Ihsan Çaha International Iberian Nanotechnology Laboratory, Braga, Portugal Title: “Advanced Transmission Electron Microscopy for Understanding Energy-Related Materials”
9.50 – 10.15	Keynote Address D. Pukazhselvan TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal Title: “Ground Analysis: Hydrogen vs Batteries for Vehicular Applications”

Session:2

Chair: Francisco Loureiro

10.15 – 10.35	Invited Talk-1 Aamer Ali Department of Energy, Aalborg University, Denmark Title: “Membrane Technology for Sustainable Energy Transition”
10.35 – 10.55	Invited Talk-2 Sivabalan Maniam Sivasankar Department of Physics, i3N, University of Aveiro, 3810-193, Aveiro, Portugal Title: “Progress in Thin-Film Photovoltaics: Emerging Strategies for High-Efficiency and Scalable Solar Energy Conversion”

10.55 – 11.15	Invited Talk-3 Parsa Behzad Nazif University of Oviedo, Spain Title: “Parameter Estimation for Digital Twin in Power Electronic Converters”
11.15 – 11.35	Invited Talk-4 Sathishkumar Duraisamy Centre for Mechanical Technology and Automation (TEMA), Department of Mechanical Engineering, University of Aveiro, Portugal. Title: “Electron Beam Welding of Copper Tubes for Heat Pump Refrigerant Circuits: Process–Property Relationships and Mechanical Performance”
11.35 – 11.45	Session break

Session:2

Chair: D. Pukazhselvan

11.45 – 12.15	Invited Talks-5 and 6 Jaykumar Lachure Department of Computer Science and Engineering, Indian Institute of Information Technology (IIIT) Sri City, Chittoor 517646, Andhra Pradesh, India Title: “Quantum-Machine Learning for Discovery of Entropy-Stabilized High-Entropy Alloy Hydrides in Ambient Hydrogen Storage” Jaykumar Lachure / Sagar Lachure Department of Computer Science and Engineering, Indian Institute of Information Technology (IIIT) Sri City, Chittoor 517646, Andhra Pradesh, India Title: “Quantum-ML Discovery of Superionic Proton Ceramic Conductors for 520 Wh/kg Battery Applications”
12.15- 12.35	Invited Talk-7 Carlos O Amorim Department of Physics and i3N, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal Title: “Impact of Dilute Ag Distribution on Sequentially Sputtered Cu(In,Ga)(Se,S)₂ Solar Cell Performance”
12.35 – 12.55	Invited Talk-8 Deepa M. J Department of Chemistry, University of Kerala, Kariavattom campus, Thiruvananthapuram. 69558, India

	<i>Title: “Interface-Engineered WO₃/Co₃O₄ Heterostructure in NiCoP Alloy Coating for Efficient Alkaline Hydrogen Evolution Reaction”</i>
12.55-13.15	Invited Talk-9 Francisco J. A. Loureiro TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal Title: “Mixed ionic and electronic conductors: fundamentals and optimisation strategies”
13.15-13.25	Vote of Thanks/Concluding remarks D. Pukazhselvan (convener) Francisco Loureiro (Co-convener)

*Fifth International workshop on “Modern Trends in Energy Research”
7 July 2026, University of Aveiro, Portugal*

Advanced Transmission Electron Microscopy for Understanding Energy-Related Materials

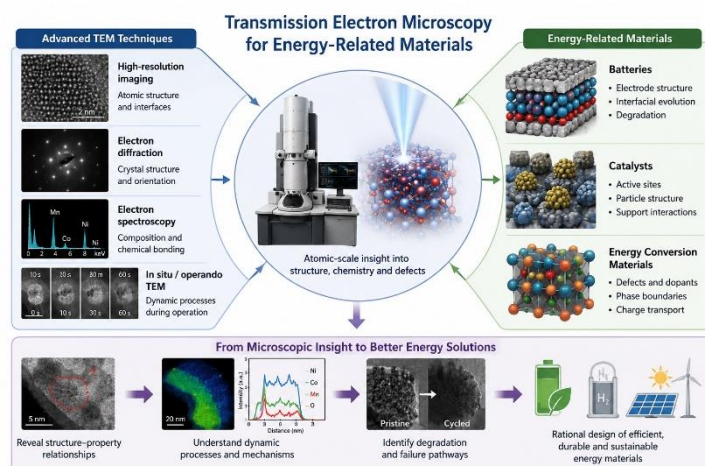
Ihsan Çaha

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Abstract:

The development of next-generation energy technologies relies on a fundamental understanding of materials across multiple length scales. Transmission electron microscopy (TEM) has become an indispensable tool for probing the structure, chemistry, and defects of energy-related materials with atomic-scale resolution. This presentation will highlight recent advances in TEM techniques, including high-resolution imaging, electron diffraction, spectroscopy, and in situ/operando microscopy, and their application to batteries, catalysts, and functional materials for energy conversion and storage. Particular emphasis will be placed on revealing structure–property relationships, dynamic processes during operation, and degradation mechanisms that limit performance. These insights provide valuable guidance for the rational design of more efficient, durable, and sustainable energy materials.



Acknowledgment: This work was supported by the Innovation Pact “NGS – New Generation Storage” (C644936001-00000045), by “NGS” Consortium, co-funded by Next Generation EU from the European Union, through the Incentive System “Agendas for Business Innovation” (“Agendas para a Inovação Empresarial”), within the Recovery and Resilience Plan (PRR).

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Ground Analysis: Hydrogen vs Batteries for Vehicular Applications

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The transportation sector is undergoing a major transition as the era of fossil-fuel-powered mobility approaches its limits due to concerns over climate change, resource depletion, and environmental sustainability. Several alternative energy carriers have emerged, including batteries, hydrogen, ammonia, and green methane [1]. Among these, batteries and hydrogen have attracted the greatest attention for vehicular applications because of their potential to enable near-zero-emission transportation. This work presents a ground-level analysis of batteries and hydrogen as competing and complementary solutions for future mobility. From an energy-density perspective, hydrogen possesses a clear advantage, offering significantly higher gravimetric energy content than current battery technologies. However, from the standpoint of technological maturity, infrastructure readiness, and overall feasibility, batteries currently hold a dominant position, particularly in passenger vehicles.

There are three key stages of the hydrogen value chain, production, storage, and end-use. Significant progress has recently been achieved in hydrogen production through solar-driven and renewable-powered routes, while advances in low-temperature fuel cells and hydrogen-fueled internal combustion engines are improving the economic viability of hydrogen utilization. Nevertheless, hydrogen storage remains the most challenging intermediate step, limiting widespread adoption despite hydrogen's exceptional energy potential. Nonetheless, recent developments in metal hydride systems suggest promising pathways toward sustainable hydrogen storage. In particular, solar-thermal-assisted hydrogen release from Cu–Ni alloy incorporated MgH₂ systems [2] has demonstrated the possibility of achieving hydrogen desorption capacities approaching 6 wt.% through in situ solar heat utilization. Such advances indicate that not only hydrogen production but also hydrogen storage may be integrated with renewable energy sources, thereby enhancing the overall sustainability of the hydrogen economy.

Acknowledgment: This article was supported by the projects 2022.09319.PTDC, 2022.02498.PTDC, UIDB/00481/2020, UIDP/00481/2020 and UIDP/50006/2020 from Fundação para a Ciência e a Tecnologia (FCT), and CENTRO-01-0145-FEDER-022083 from Centro Portugal Regional Operational Programme (Centro2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund (ERDF). Author acknowledge FCT, Portugal for the financial support with reference CEECIND/04158/2017.

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W1-I1. Membrane Technology for Sustainable Energy Transition

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Membrane technologies offer energy-efficient and scalable solutions to support the transition toward a sustainable energy future. This presentation highlights some of the activities we are currently undertaking in our laboratory on membrane-based processes for green hydrogen production, carbon capture, and battery recycling. Membrane distillation is being developed to produce ultrapure water from alternative water sources, enabling sustainable hydrogen generation through integrated membrane–electrolyzer systems. In parallel, membrane contactors are being investigated as compact and modular technologies for CO₂ capture, building on extensive expertise in water treatment membrane processes to optimize performance and facilitate scale-up. The presentation also covers our activities on membrane technologies applied in battery recycling to enhance the selective recovery of critical materials and support circular resource utilization. Overall, the presentation highlights the pivotal role of membrane processes in addressing interconnected challenges of water, energy, carbon management, and resource recovery, thereby contributing to a low-carbon and resource-efficient energy system.

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W1-I2. Progress in Thin-Film Photovoltaics: Emerging Strategies for High-Efficiency and Scalable Solar Energy Conversion

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The continued expansion of renewable energy technologies has intensified the search for photovoltaic solutions capable of combining high conversion efficiency, reduced material consumption, scalable manufacturing, and long-term sustainability. Among the available photovoltaic technologies, thin-film solar cells have emerged as promising alternatives to conventional crystalline silicon due to their lower absorber thickness, compatibility with large-area processing, and potential for reduced production costs [1]. In recent years, substantial advances have been achieved across multiple thin-film platforms through the integration of interface engineering, compositional optimization, defect control, and novel processing approaches [1].

Drawing from recent developments across the field, attention has increasingly focused on three major thin-film photovoltaic technologies—Cu(In,Ga)Se₂ (CIGS), CdTe, and Cu₂ZnSn(S,Se)₄ (CZTSSe)—with emphasis on the strategies that have enabled continuous improvements in device efficiency and functional stability [1]. Particular attention is given to the relationship between material design and device performance, highlighting how microstructural control, interface passivation, band alignment optimization, and absorber engineering influence charge carrier transport and recombination dynamics [1].

Among these technologies, CIGS remains one of the most mature and high-performing thin-film absorbers due to its tunable bandgap, strong optical absorption, and demonstrated laboratory-scale efficiencies exceeding 23% [1], [2]. Recent developments have focused on alkali-assisted growth, compositional grading, surface and interface passivation, and precursor engineering to suppress recombination losses and improve open-circuit voltage [1]. These developments align closely with current research directions aimed at understanding and tailoring interfacial phenomena within chalcopyrite absorber systems to further enhance carrier collection and overall device performance [1].

In parallel, CdTe technology continues to benefit from advances in defect management, contact engineering, and optimized post-deposition treatments that improve charge extraction and long-term reliability [1]. Meanwhile, CZTSSe remains attractive as an earth-abundant and environmentally conscious alternative, where ongoing efforts concentrate on mitigating defect-related limitations, reducing secondary phases, and improving grain growth and interface quality [1].

Beyond efficiency enhancement, current developments in thin-film photovoltaics increasingly consider broader challenges related to sustainability, scalability, material availability, and industrial deployment [1]. Emerging directions involving multifunctional interfaces, advanced characterization techniques, and integrated processing approaches continue to expand opportunities for improving both performance and manufacturability in next-generation solar energy technologies [1].

Overall, continued progress in thin-film photovoltaics is expected to depend not only on improvements in absorber quality but also on increasingly precise control of interfaces and defect landscapes across multiple length scales [1]. Advances in these areas reinforce the potential of thin-film technologies to contribute

meaningfully to future energy systems through efficient, scalable, and economically viable solar energy conversion [1].

Acknowledgment: *This research was funded by FEDER funds through the COMPETE 2020 Program and National Funds through FCT—Portuguese Foundation for Science and Technology under the projects LISBOA-01-0247-FEDER-039985/POCI-01-0247-FEDER-039985, LA/P/0037/2020, UIDP/50025/2020, and UIDB/50025/2020 of the Associate Laboratory Institute of Nanostructures, Nanomodelling and Nanofabrication—i3N.*

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*Fifth International workshop on “Modern Trends in Energy Research”
7 July 2026, University of Aveiro, Portugal*

W1-I3. Mixed ionic and electronic conductors: fundamentals and optimisation strategies

Allan J. M. Araújo^{1,2}, Vanessa C. D. Graça^{1,2}, Laura I. V. Holz^{1,2}, Duncan P. Fagg^{1,2},

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² LASI - Intelligent Systems Associate Laboratory, 4800-058, Guimarães, Portugal

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

Acknowledgment: This work is funded by national funds through FCT – Fundação para a Ciência e a Tecnologia, I.P., under the project/contract UID 00481 - Centre for Mechanical Technology and Automation, as well as the following grants/projects: 2020.02797.CEECIND/CP1589/CT0030, 2023.05868.CEECIND/CP2840/CT0021, 2024.08832.CEECIND, 2022.02498.PTDC, 2022.09319.PTDC, 2024.14251.PEX, 2022.09319.PTDC, 2024.14251.PEX, and UID 00481/2025 – Centre for Mechanical Technology and Automation (<https://doi.org/10.54499/2020.02797.CEECIND/CP1589/CT0030>), (<https://doi.org/10.54499/2023.05868.CEECIND/CP2840/CT0021>), (<https://doi.org/10.54499/2022.02498.PTDC>), (<https://doi.org/10.54499/2022.09319.PTDC>), (<https://doi.org/10.54499/2024.14251.PEX>), and UID 00481/2025 – Centre for Mechanical Technology and Automation (<https://doi.org/10.54499/UID/00481/2025>). Acknowledgement is also given to COMPETE 2030 for the following projects: COMPETE2030-FEDER-00744500 16284 2023.17866.ICDT (<https://doi.org/10.54499/2023.17866.ICDT>), COMPETE2030-FEDER-00770000 16527 2023.17134.ICDT, and COMPETE2030-FEDER-00820300 16919 2023.18516.ICDT.

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*Fifth International workshop on “Modern Trends in Energy Research”
7 July 2026, University of Aveiro, Portugal*

W1-I4. Electron Beam Welding of Copper Tubes for Heat Pump Refrigerant Circuits: Process–Property Relationships and Mechanical Performance

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Abstract: Copper tube connections in heat pump refrigerant circuits must remain leak-proof throughout their service life, enduring continuous thermal cycling and mechanical vibrations. However, improved joining processes for copper in such thermal management systems are still needed [1]. Brazing, the conventional method, relies heavily on manual skill, carries a significant risk of human-induced defects, and involves substantial energy consumption and gas emissions, which are increasingly difficult to justify in sustainable manufacturing. Electron beam welding (EBW) directly addresses these limitations as a fully autogenous, vacuum-based process that eliminates the need for filler materials and flux, precisely controls heat input, and operates without open-flame emissions. However, copper’s high thermal conductivity narrows the EBW process window, and the relationship between welding parameters and joint performance in tubular overlap geometries remains poorly understood. This study maps the process–property relationships for EBW of Cu-DHP copper tube joints across a systematic matrix of beam currents and rotation speeds at a fixed accelerating voltage. Joints were evaluated through tensile testing, Vickers microhardness profiling, backscattered electron scanning electron microscopy (BSE-SEM), and energy-dispersive X-ray spectroscopy (EDX). Above a clear beam-current threshold, regardless of welding speed, three distinct regimes emerge: a no-bond conduction regime characterised by brittle interfacial failure; a partial-fusion transitional regime exhibiting moderate strength and ductility; and a stable full-keyhole regime, in which the optimal condition achieved a joint efficiency of 86% relative to the base metal. BSE-SEM revealed a progressive evolution from an intact oxide interface through columnar dendrites to a fine equiaxed solidification structure within the fusion zone, while EDX analysis confirmed that full keyhole conditions markedly reduce oxygen at the bond line through melt-pool convection that expels surface oxides and directly improves leak resistance. Microhardness profiles indicate a consistently harder fusion zone than the surrounding heat-affected zone, with the extent of softening determined by the local heat input. These results reveal a clear parameter hierarchy: beam current governs the fusion mode and thus determines the achievable joint quality, while rotation speed serves as a secondary variable that fine-tunes performance within the regime set by the beam current. Only once the correct current level is reached does speed optimisation become meaningful, providing a direct and practical framework for parameter selection in heat pump copper tube manufacturing, where consistent leak integrity and joint strength must be achieved without the environmental impact of conventional brazing.

Acknowledgement: *This work was supported by Fundação para a Ciência e a Tecnologia, I.P., through grant 2025.06480.BD and under project/contract UID 00481 – TEMA.*

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**W1-I5. Quantum-Machine Learning for Discovery of Entropy-Stabilized
High-Entropy Alloy Hydrides in Ambient Hydrogen Storage**

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Abstract: The global energy transition toward hydrogen systems is limited by the lack of practical solid-state storage. Conventional metal hydrides face a thermodynamic trade-off: strong binding gives high capacity but requires desorption above 150 °C, while weak binding supports ambient operation but with < 2 wt% capacity. High-entropy alloy hydrides overcome this limitation through entropy engineering [1], where configurational entropy shifts the van’t Hoff equilibrium into the 1–10 bar range at 25–100 °C without changing formation enthalpy. To search the vast composition space, we use a three-stage quantum-ML framework: (1) VQE on 8–12 qubit clusters achieves enthalpy errors of 1.5 kJ/mol, outperforming DFT; (2) a QGAN generates targeted compositions; and (3) equivariant GNNs such as NequIP and MACE predict enthalpies with MAE below 2.8 kJ/mol [2]. Active learning converges in 15 iterations. The framework identifies TiZrNbHf-based HEAHs as leading candidates. The top composition, Mg_{0.2}Ti_{0.2}Fe_{0.2}Ni_{0.2}Co_{0.2}-H, delivers 5.7 wt% capacity at 25 °C with a 2.8 bar plateau pressure and 98% retention after 100 cycles [3]. It remains structurally stable from -40 °C to 100 °C and shows no XRD degradation, with a heat of formation of -28.5 kJ/mol H₂. Techno-economic analysis projects \$6–8/kWh, meeting DOE 2025 targets. This work establishes entropy-stabilized HEAHs as a viable route for ambient-temperature hydrogen storage and shows how quantum-ML can accelerate discovery in high-dimensional materials spaces [4].

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**W1-I6. Quantum-ML Discovery of Superionic Proton Ceramic Conductors
for 520 Wh/kg Battery Applications**

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Abstract: Solid-state lithium-ion batteries are approaching their ~300 Wh/kg theoretical limit, necessitating new battery chemistries. Proton-conducting ceramics offer a different paradigm by shuttling H⁺ through oxide lattices rather than lithium ions, eliminating lithium entirely and relying on earth-abundant barium, zirconium, and oxygen [1]. However, proton conductivity of state-of-the-art acceptor-doped perovskites (10⁻³–10⁻² S/cm at 300°C) remains >10× below the 0.1 S/cm threshold for practical battery operation. Here, we demonstrate coherent quantum tunneling of protons between adjacent oxygen sites boosts ionic conductivity by two orders of magnitude when lattice geometry creates resonant tunneling conditions. We employ Quantum Imaginary Time Evolution (QITE) on trapped-ion quantum computers (IonQ Forte, Quantinuum H2) to compute proton ground-state energies in doped perovskite clusters with 2% ZPE accuracy, vs. 15–40% systematic underestimation of DFT [2]. A transformer neural network trained on 2,000 quantum-computed proton transfer barriers predicts conductivity for 10,000 perovskite compositions [3], identifying BaZr_{0.5}Sc_{0.3}Y_{0.2}O₃ as the optimal composition with predicted proton conductivity of 0.15 S/cm at 300°C, exceeding the battery threshold. The resulting H₂ | BaZr_{0.5}Sc_{0.3}Y_{0.2}O₃ | O₂ full cell achieves **520 Wh/kg with 92% round-trip efficiency** and cycle life exceeding **12,000 cycles**, establishing an entirely new battery chemistry beyond lithium at a projected cost of **\$20/kWh** using earth-abundant precursors [4]. These results establish a new era of quantum-accelerated materials design for high-performance electrochemical energy storage.

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W1-I7. Impact of Dilute Ag Distribution on Sequentially Sputtered Cu(In,Ga)(Se,S)₂ Solar Cell Performance

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Abstract: Cu(In,Ga)(Se,S)₂ (CIGSSe) is a leading thin-film photovoltaic material due to its high absorption coefficient, tunable bandgap, and compatibility with lightweight and scalable solar technologies. Ag alloying has emerged as a promising strategy to improve this absorber growth and electronic quality, but most studies have focused on co-evaporated absorbers and relatively high Ag contents. Here, we show that in sequentially sputtered CIGSSe absorbers, very low Ag incorporation can still produce substantial performance gains, provided that its vertical distribution is carefully controlled. This is particularly relevant for cost-effective and industrially scalable solar energy materials [1-4].

Three absorber configurations were prepared on soda-lime glass/Mo substrates using sequential deposition of metallic precursors followed by rapid thermal processing in an S-rich atmosphere: an Ag-free reference (CIGS-R), a uniformly Ag-alloyed absorber (ACIGS-F), and a partially Ag-alloyed absorber with Ag introduced only in the upper half of the precursor stack (ACIGS-P). The overall Ag/(Ag+Cu) ratio was kept low, at about 3.0–3.5 at.%. After absorber formation, devices were completed with CdS/i-ZnO/ITO front layers.

XRD confirmed chalcopyrite phase formation in all samples with no detectable secondary phases. Ag incorporation promoted grain growth in both Ag-containing absorbers, with ACIGS-F showing the largest grains and densest morphology. However, this sample also exhibited the worst device performance, with $V_{oc} = 412$ mV, $J_{sc} = 23.6$ mA.cm⁻², FF = 38.0%, and PCE = 3.7%.

In contrast, ACIGS-P delivered the best overall performance, reaching $V_{oc} = 525$ mV, $J_{sc} = 33.6$ mA.cm⁻², FF = 64.4%, and PCE = 11.3%, compared with 7.1% for the Ag-free reference.

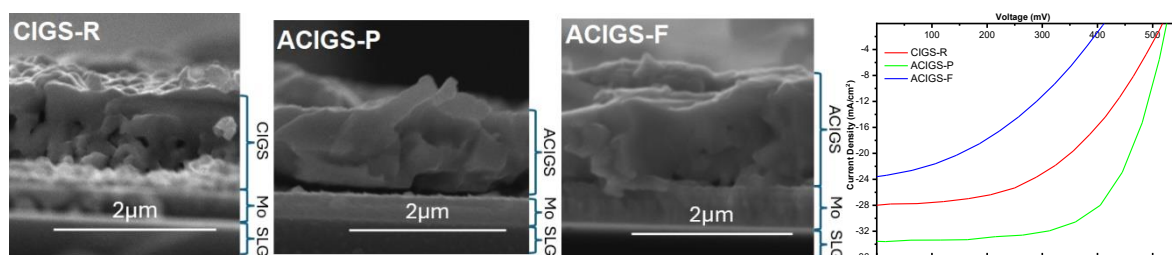


Fig. 1 (left) SEM micrographs of the cross section of CIGS-R, ACIGS-P and ACIGS-F. (right) J-V curves of all samples.

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**W1-I8. Interface-Engineered WO₃/Co₃O₄ Heterostructure in NiCoP Alloy
Coating for Efficient Alkaline Hydrogen Evolution Reaction**

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The development of Nickel-based electrocatalysts is critical for realizing efficient, scalable, and economically viable hydrogen production through water splitting. In the present study, a novel approach utilizing electroless NiCoP coating is employed to develop WO₃/Co₃O₄ incorporated NiCoP coating with tunable compositions. The prepared WO₃/Co₃O₄ composite exhibits sharp diffraction peaks of monoclinic WO₃ and cubic spinel Co₃O₄, confirming the successful formation of the WO₃/Co₃O₄ composite. The prepared WO₃/Co₃O₄ composite shows enhanced absorption edges with redshift and low PL intensity due to the successful formation of a heterojunction between Co₃O₄ and WO₃, which confirms the enhanced catalytic performance of the prepared composite. Also, the large surface area and the pore volume of the prepared WO₃/Co₃O₄ composite obtained from BET analysis supports the enhanced catalytic performance. The effective incorporation of WO₃/Co₃O₄ composite into the NiCoP coating is confirmed through morphological and compositional analyses. The optimized WO₃/Co₃O₄@NiCoP coating exhibits lower charge transfer resistance (28.67 Ω cm²), reduced overpotential (-115 mV/dec at 10 mA/cm²) and Tafel slope (102 mV/dec) than other coatings, confirming the enhanced electrocatalytic performance of the coating. From the results, it is confirmed that the developed coating could serve as an efficient electrocatalyst for HER, contributing to the development of sustainable energy technologies via water electrolysis. From the results, a plausible mechanism of the electrocatalytic HER over the developed coating in alkaline media is proposed.

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**W1-I9. Parameter Estimation for Digital Twin in Power Electronic
Converters**

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Accurate parameter estimation is essential for developing reliable digital twins of power electronic converters. Electrical parameters such as inductance, capacitance, equivalent series resistance, and semiconductor on-state resistance vary with temperature, aging, and operating conditions, causing deviations between the physical system and its digital representation. By identifying these parameters online or offline, parameter estimation improves model accuracy, enhances control performance, and enables condition monitoring and predictive maintenance, contributing to more intelligent and resilient power electronic systems.

Acknowledgment: *This work was supported in part by the European Commission’s HORIZON and KDTJU programs through the project POWERIZED under Grant 101096387, in part by the Spanish Ministry of Science and Innovation under Grant MCINN-23-PCI2022-135021-2, and in part by the Government of the Principality of Asturias under Project SEK-25-GRU-GIC-24-023.*

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3rd Workshop on High Valued Developments in Photocatalysis



International Workshop on High Valued Developments in Photocatalysis [HVDP-2026]

The PGK Mandal's Haribhai V. Desai College of Arts, Science &
Commerce (Autonomous) Pune, India

Tuesday, 07th July, 2026

Time: 1:30 PM [IST]



International Workshop on High Valued Developments in Photocatalysis (HVDP-2026)

The PGK Mandal's Haribhai V. Desai College

of Arts, Science & Commerce (Autonomous) Pune, India

Thursday, 7th July 2026 1:30PM (IST), 9 AM (PT)

The Poona Gujarati Kelavani Mandal's H. V. Desai College is recognized as one of the premier academic institutions in Pune city. It stands tall in public esteem and in the memories of its alumni, many of whom are now prominent figures in the government, business and industry, media and education sector. Students from all backgrounds have grown and excelled in the chosen areas of their interests; be it academics, sports or extra-curricular activities. H. V. Desai College was established in 1984, by The Poona Gujarati Kelvani Mandal. It started as an organization to cater to the Gujarati minority and the traditional business sections of the society. This promoted education and motivated especially girl students in vicinity to pursue higher education. The college is declared an autonomous college from year 2024-25.

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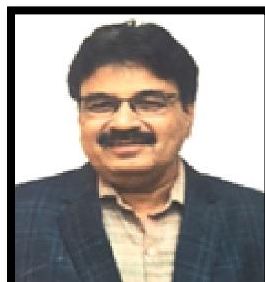


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HVDP-2026 Program

Auditorium 2 International Workshop on High Valued Developments in Photocatalysis [HVDP-2026] The PGK Mandal's Haribhai V. Desai College of Arts, Science & Commerce (Autonomous) Pune, India Tuesday, 07th July, 2026	
9:30–9:35	Welcome by Dr. Vikram Pandit and Dr. Prakash P. Wadgaonkar
9:35–9:40	Inauguration by Principal Dr. Rajendra G. Gurao and Dr. Prakash P. Wadgaonkar
9:40–10:00	Session Chair: Dr. Vikram Pandit Invited Talk Dr. Gustava Colpani (W2-I1) Community University of Chapecó Region – UNOCHAPECÓ Title: “Heterogeneous Photocatalysis: Fundamentals and Applications”
10:00–10:20	Invited Talk Dr. Yashpal Rathod (W2-I2) Department of Chemistry, J. M. Patel College of Science, Bhandara (M.S.) INDIA Title: “SYNTHESIS, CHARACTERIZATION AND PHOTOLUMINESCENCE APPLICATION OF SALICYLIC ACID-PHENYL HYDRAZINE FORMALDEHYDE-CHARCOAL COMPOSITE”
10:20–10:30	Oral Talk Ganesh Dawange (W2-O1) Haribhai V. Desai College, Pune, India Title: “Medicinal Plant-Derived CuO Nanostructures: Visible-Light Photocatalysis and Antibacterial Potential”
10:30–10:40	Oral Talk Sonali Nikam (W2-O2) Research Centre, Department of Chemistry, MGV. M.S.G.Arts, Science, and Commerce College, Malegaon. (MH), India-423105 Title: “Synthesis of Fe₂O₃-SnO₂ Nanocomposites for Photocatalytic EBT Dye Degradation”

10:40–10:50	Oral Talk Ganesh Jadhav (W2-O3) Department of Chemistry, The PGK Mandal's Haribhai V. Desai College of Arts Science and Commerce (Autonomous), Pune-411002, India Title: "Tailored Pr (OH)₃ Nanomaterial for Photocatalysis and Antimicrobial Performance"
10:50–11:00	Oral Talk Abhijit Sonone (W2-O4) Modern College, Shivajinagar, Pune, India Title: "Synthesis of Graphene-Based Nanocomposites for Water Purification"
11:00–11:10	Oral Talk Tushar Patil (W2-O5) Dr. Yusuf Hamied Department of Chemistry, Ramnarain Ruia Autonomous College, Mumbai 400019, India Title: "ZrO₂@S-doped g-C₃N₄ hybrid Nanocomposites for Enhanced Dye Adsorption for MB and MO"
11:10–11:20	Oral Talk Sahebrao Dolnar (W2-O6) Dr. Yusuf Hamied Department of Chemistry, Ramnarain Ruia Autonomous College, Mumbai 400019, India Title: "Synergistic effects of α-MnO₂ on the structural, optical and Photocatalytic properties of ZnFe₂O₄"
11:20–11:30	Oral Talk Vinícius Tres Orso (W2-O7) Community University of Chapecó Region - UNOCHAPECÓ, Servidão Anjo da Guarda, 295-D, Chapecó, Santa Catarina, Brazil Title: "Development of Titanium Electrodes Modified with Polypyrrole and Niobium for the Photoelectrocatalytic Degradation of Tetracycline and Tramadol"

11:30–11:40	Oral Talk Bhagwan Daphal (W2-O8) Department of Chemistry, Haribhai V. Desai College of Commerce, Arts and Science, Pune-411002, India <i>Title: “Synthesis and Characterization of Polyaniline Vanadium Pentoxide nanocomposite for Photocatalytic Degradation of Organic Pollutants”</i>
11:40–11:50	Oral Talk Priyanka Bhalerao (W2-O9) Dr. T. R. Ingle Research Laboratory, Department of Chemistry, S. P. College, Pune–30, India <i>Title: “Controlled Hydrothermal Synthesis of CoS₂ Microspheres toward Multifunctional Energy and Biological Applications”</i>
11:50–12:00	Vote of Thanks/Concluding remarks



*International Workshop on High Valued Developments
in Photocatalysis
The PGK Mandal's Haribhai V. Desai College of Arts,
Science & Commerce (Autonomous)
Pune, India, 7 July, 2026*

Invited Talk

W2-I1. Heterogeneous Photocatalysis: Fundamentals and Applications

Colpani, Gustavo Lopes

Community University of Chapecó Region – UNOCHAPECÓ

Most conventional wastewater treatment technologies are non-destructive toward many contaminants, acting primarily by removing them from the aqueous matrix through adsorption or coagulation/physical separation. As a result, these processes generate a solid residue that is difficult to treat, in which the pollutants remain concentrated, having merely undergone a phase transfer. In contrast, Advanced Oxidation Processes (AOPs) have emerged as an efficient, versatile, and cost-effective alternative, operating under mild temperature and pressure conditions while achieving high mineralization rates of organic pollutants, thereby representing a more environmentally sustainable treatment option. Their principle is based on the generation of highly reactive oxidative species, including hydroxyl radicals ($\bullet\text{OH}$), singlet oxygen ($^1\text{O}_2$), and superoxide radicals (O_2^-), which promote the degradation of complex organic compounds. This degradation initially leads to the formation of intermediate by-products, yielding organic species of lower molecular complexity, and may ultimately result in the complete mineralization of contaminants into carbon dioxide (CO_2), water (H_2O), and inorganic salts, particularly in the presence of nitrogen-, sulfur-, or chlorine-containing compounds. Among the AOPs capable of generating these reactive species, Fenton processes, heterogeneous photocatalysis, ozonation, photolysis, sonolysis, and electrochemical oxidation are particularly noteworthy. In this context, this presentation will discuss the fundamental concepts of heterogeneous photocatalysis, and the mechanisms involved in hydroxyl radical generation, as well as selected strategies developed by our research group to enhance the photocatalytic activity of semiconductor materials.

Invited Talk

**W2-I2. SYNTHESIS, CHARACTERIZATION AND
PHOTOLUMINESCENCE APPLICATION OF SALICYLIC ACID-
PHENYL HYDRAZINE FORMALDEHYDE-CHARCOAL COMPOSITE**

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Salicylic acid-phenyl hydrazine formaldehyde-charcoal composite were synthesized by ultrasonication method using salicylic acid-phenyl hydrazine formaldehyde (SPHF-I) copolymer and activated charcoal in 1: 2 molar ratios and DMSO as a solvent. The SPHF-I copolymer were first synthesized using salicylic acid, phenyl hydrazine and formaldehyde as a monomer in 1:1:2 molar ratios by polycondensation polymerization method in presence of 2M HCl was used as an acid catalyst at 122⁰C. The synthesized copolymer and composite were characterized by using UV-visible, FTIR and scanning electron microscopy. The thermogravimetric analysis were carried out to determine kinetic and thermodynamic parameters using Sharp-Wentworth and Freeman-Carroll method. Based on the TGA data activation energy obtained by both this method is good agreement with each other and low value of frequency factor indicate slow degradation of the copolymer and composite. From the value of the order of reaction it shows that copolymer and composite follows first-order kinetics. The photoluminescence study of synthesized composite was carried out using the RF-501 (PC) S CE (LVD) MODEL PL spectrometer.

W2-O1. Medicinal Plant-Derived CuO Nanostructures: Visible-Light Photocatalysis and Antibacterial Potential

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A promising method for the removal of pollutants and the disinfection of water is a green approach to complex CuO photocatalysts. We present a plant-extract-mediated precipitation-calcination strategy that employs aqueous leaf extracts of *Mitragyna parviflora* and *Leptadenia reticulata* to direct CuO growth from granular nanoparticles into distinct fused-prism nanostructures (CMP and CLR). X-ray diffraction confirms the presence of phase-pure monoclinic CuO in all samples, while FESEM/TEM demonstrates the progression from irregular aggregates (extract-free CuO) to faceted plates (CMP) and densely interlocked prisms (CLR). The band-gap is observed to narrow from 2.32 eV (CuO) to 1.35-1.36 eV (CMP, CLR) in diffuse reflectance spectroscopy. This is accompanied by photoluminescence quenching and subtle changes in the X-ray photoelectron spectra of Cu 2p and O 1 s, which suggest alterations in the structure of the defect and the speciation of surface oxygen. In natural sunlight, CLR exhibits the highest photocatalytic activity for Rhodamine 6 G, methylene blue, and safranin, with apparent rate constants of up to $9.81 \times 10^{-3} \text{ min}^{-1}$. Also it improves the degradation of 4-chlorophenol as compared to extract-free CuO and CMP. In agar well diffusion assays against *Escherichia coli* (EC), *Pseudomonas aeruginosa* (PA) and *Staphylococcus aureus* (SA), the plant-derived samples, particularly CLR, showed significantly larger inhibition zones and strong antibacterial activity. The structure and defects of CuO are guided by medicinal plant extracts to form fused-prism architectures, which improve the antibacterial and visible-light photocatalytic performance.

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W2-O2. Synthesis of $\text{Fe}_2\text{O}_3\text{-SnO}_2$ Nanocomposites for Photocatalytic EBT Dye Degradation

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In light of their toxicity, durability, and resistance to traditional wastewater treatment techniques, the growing discharge of synthetic dyes from textile and industrial effluents poses a major hazard to aquatic ecosystems and human health. Semiconductor-based photocatalysis has become one of the most efficient and eco-friendly advanced oxidation methods for the breakdown of organic contaminants. Energy-dispersive X-ray spectroscopy (EDS) for elemental analysis, Fourier-transform infrared spectroscopy (FTIR) for functional group identification, scanning electron microscopy (SEM) for surface morphology, and X-ray diffraction (XRD) for phase composition and crystallinity were used to characterise the synthesised nanocomposites, and UV-visible spectroscopy to assess band gap energy and optical characteristics. Eriochrome Black T (EBT) dye degradation under light irradiation was used to test the photocatalytic efficiency of the $\text{Fe}_2\text{O}_3\text{-SnO}_2$ nanocomposite. Degradation efficiency was rigorously assessed in relation to catalyst dose, starting dye concentration, solution pH, and irradiation period. Due to the creation of a heterojunction that efficiently inhibits electron-hole recombination and encourages the production of reactive oxygen species, the $\text{Fe}_2\text{O}_3\text{-SnO}_2$ composite demonstrated noticeably higher photocatalytic activity than the individual metal oxides. The degradation kinetics showed quick and effective EBT dye elimination, following a pseudo-first-order model. These results suggest that $\text{Fe}_2\text{O}_3\text{-SnO}_2$ composite nanoparticles are suitable photocatalysts for the treatment of wastewater polluted with dyes and provide a long-term solution for environmental remediation.

W2-O3. Tailored Pr (OH)₃ Nanomaterial for Photocatalysis and Antimicrobial Performance

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Praseodymium hydroxide (Pr (OH)₃) nanorods were synthesized via a hydrothermal method and extensively analysed for their photocatalytic and antibacterial properties. X-ray diffraction confirmed the hexagonal crystal structure, whereas FTIR analysis substantiated the formation of Pr–O bonds. SEM imaging revealed uniform, well-defined nanorods of 100–150 nm in length and 20–30 nm in diameter. Upon assessment of photocatalytic efficiency under solar irradiation, the nanorods achieved the destruction of 30% of Rhodamine 6G ($k = 6.09 \times 10^{-3} \text{ min}^{-1}$) and 10% of Crystal Violet ($k = 1.53 \times 10^{-3} \text{ min}^{-1}$) over a 60-minute period. Antimicrobial efficacy was demonstrated against Escherichia coli and Staphylococcus aureus, with inhibition zones of 4 mm and 6 mm, respectively. The stability and recyclability of Pr(OH)₃ highlight its potential for environmental remediation and biological applications. Future endeavour's will focus on optimizing synthesis parameters and developing composite nanomaterials to enhance performance.

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W2-O4. Synthesis of Graphene-Based Nanocomposites for Water Purification

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Water pollution resulting from industrialisation and urbanisation has become a serious global problem, which has created an immediate demand for sophisticated, effective and sustainable water treatment solutions. Graphene oxide (GO)-based ternary nanocomposites have drawn extensive interest as promising materials for water purification due to their distinctive physicochemical properties and multifunctional features. This study reviews in depth the synthesis, characteristics, performance improvement and environmental applications of GO based ternary nanocomposites. Due to its huge surface area, large number of oxygen-containing functional groups, and great dispersibility, GO is a perfect platform for the construction of hybrid nanocomposites. The synergistic interaction between the metal or metal oxide and Sulphide parts with a third functional material enhances the adsorption capacity, photocatalytic efficiency and antibacterial activity. They covered different ways of synthesis such as GO preparation by Improved Hummers' method and fabrication of nanocomposites by hydrothermal, sol-gel, co-precipitation and green synthesis methods. The water purification techniques include adsorption, photocatalysis and antibacterial activity that enable the effective removal of heavy metals, dyes, organic contaminants and pathogens. Methods to increase the performance such as band gap adjustment, heterojunction creation and surface modification can further enhance the efficiency and stability. The paper also discusses the broad spectrum of environmental applications of these nanocomposites in the area of water purification and water disinfection. However, toxicity, environmental effect, cost, scalability and material recovery problems are still significant issues for real life applications. Future research should focus on sustainable synthesis, better recyclability and thorough risk evaluation for safe and large-scale use of these materials.

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*3rd International Workshop on High Valued Developments in Photocatalysis
The PGK Mandal's Haribhai V. Desai College of Arts, Science & Commerce (Autonomous)
Pune, India, 7 July, 2026*

W2-O5. ZrO₂@S-doped g-C₃N₄ hybrid Nanocomposites for Enhanced Dye Adsorption for MB and MO

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Graphitic carbon nitride (g-C₃N₄) was produced through high-temperature calcination of Thiourea. Its adsorption capabilities were assessed by tracking the uptake of Methylene blue and Methyl orange. The hybrids exhibited markedly higher adsorption capacity than pure g-C₃N₄ or ZrO₂. A comprehensive characterization involved X-ray diffraction (XRD), scanning electron microscopy (SEM), UV–vis diffuse reflectance spectroscopy (DRS), Fourier transform infrared spectroscopy (FT-IR) and particle size analysis (Zeta potential analysis). The ZrO₂@S-doped g-C₃N₄ hybrid nanocomposite was designed to improve dye removal through the combined advantages of its constituents. Sulfur-doped g-C₃N₄ offers a defect-rich, high–surface-area framework with abundant nitrogen sites that favor strong interaction with cationic methylene blue, while ZrO₂ contributes surface hydroxyl groups and positively charged sites that enhance adsorption of anionic methyl orange. The close interfacial integration increases available active sites, limits material agglomeration, and optimizes surface charge characteristics, leading to efficient adsorption of both dyes with good stability and reusability in aqueous systems.

W2-O6. Synergistic effects of α - MnO_2 on the structural, optical and Photocatalytic properties of ZnFe_2O_4

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In this study, α - MnO_2 @ ZnFe_2O_4 nanocomposites were fabricated via an ultrasonication method to evaluate the influence of α - MnO_2 incorporation on the structural, optical, and photocatalytic behavior of ZnFe_2O_4 . Prepared samples were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), UV–vis diffuse reflectance spectroscopy (DRS), Fourier transform infrared spectroscopy (FT-IR). XRD analysis confirmed the coexistence of the cubic spinel ZnFe_2O_4 and tetragonal α - MnO_2 crystalline phases, indicating the successful formation of the nanocomposite. FESEM and EDX observations revealed a well-dispersed microstructure with uniform distribution of the constituent phases and improved interfacial contact. Optical characterization using UV–DRS demonstrated stronger absorption in the visible-light region along with a decrease in the optical band gap, which is beneficial for enhanced light harvesting. Overall, the synthesized α - MnO_2 @ ZnFe_2O_4 nanocomposites exhibit significant potential as visible-light-active photocatalysts for wastewater treatment and environmental remediation.



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W2-O7. Development of Titanium Electrodes Modified with Polypyrrole and Niobium for the Photoelectrocatalytic Degradation of Tetracycline and Tramadol

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The occurrence of contaminants of emerging concern (CECs) in aquatic environments and wastewater, particularly pharmaceuticals such as tetracycline and tramadol, has attracted increasing attention in recent years due to their environmental persistence, ecotoxicological potential, and resistance to conventional treatment processes, highlighting the need for advanced removal technologies. Among these technologies, photoelectrocatalysis (PEC) has emerged as a promising approach, as it in situ generates highly reactive radical species through the synergistic combination of photocatalysis and electrochemistry. Furthermore, PEC performance is strongly influenced by electrode material properties, making surface modification an attractive strategy for developing highly active, cost-effective electrodes. Among the materials employed for thin-film fabrication, niobium-based compounds and conductive polymers, such as polypyrrole (PPy), have received considerable attention owing to their catalytic and electrochemical properties. In this context, the present study aimed to develop thin-film PPy electrodes modified with niobium and electrodeposited onto titanium substrates for the photoelectrocatalytic degradation of tetracycline and tramadol in aqueous media. Initially, PPy electrodes were prepared by electropolymerization using three different approaches: unmodified PPy, co-deposition with Nb₂O₅ (0.05 M), and co-deposition with NbCl₅ (0.05 M). Based on preliminary degradation experiments, the PPy/NbCl₅ configuration was selected for optimization through a full 2³ factorial experimental design with triplicate center points. The investigated parameters were the monomer concentration in the precursor solution (0.1–0.3 M), the electropolymerization potential (0.7–0.8 V), and the electropolymerization time (30–60 s), which were established based on preliminary cyclic voltammetry and chronoamperometry studies. The NbCl₅ concentration was kept constant at 0.05 M. The electrode exhibiting the highest methylene blue (MB) degradation efficiency was obtained under condition H (0.8 V, 0.3 M, 60 s), achieving a removal efficiency of $55.67 \pm 3.33\%$ after 300 min at an applied potential of 1.0 V, as determined by cyclic voltammetry. The resulting statistical model showed excellent agreement with the experimental data ($R^2 = 0.9528$), demonstrating a satisfactory predictive capability. The optimized electrode was subsequently evaluated for the degradation of tetracycline and tramadol, with concentrations monitored by liquid chromatography–mass spectrometry (LC–MS). Applied potentials of 1.2 V and 1.4 V, respectively, were selected based on cyclic voltammetry. Complete degradation of tetracycline was achieved within 180 min, whereas tramadol exhibited a removal efficiency of only $15.69 \pm 0.80\%$ after 300 min. These findings demonstrate the potential of PPy/NbCl₅-modified titanium electrodes for the photoelectrocatalytic degradation of contaminants of emerging concern in aqueous media and indicate that simple electrodeposition strategies can contribute to the development of promising, low-cost electrode materials for advanced wastewater treatment.

W2-O8. Synthesis and Characterization of Polyaniline Vanadium Pentoxide nanocomposite for Photocatalytic Degradation of Organic Pollutants

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The nanocomposite polyaniline (PANI)/vanadium pentoxide (V_2O_5) successfully produced in situ chemical oxidative polymerization approach. The structural, morphological, and optical characteristics of the synthesized materials were systematically characterized using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), UV-visible diffuse reflectance spectroscopy (UV-Vis DRS) and photoluminescence (PL) spectroscopy. The photocatalytic activity was measured using the degradation of Rhodamine 6G dye under visible light irradiation. With almost 70% degradation in 120 minutes, the PANI/ V_2O_5 nanocomposite showed remarkable photocatalytic performance. The synergistic interaction between conducting PANI and semiconducting V_2O_5 , which promotes efficient separation and migration of photogenerated charge carriers and increases the formation of reactive oxygen species ($\bullet OH$ and $\bullet O_2^-$) responsible for pollutant mineralization, is responsible for this enhanced photocatalytic performance. Furthermore, the nanocomposite showed exceptional structural stability and reusability after multiple photocatalytic cycles, indicating its suitability for long-term applications.

W2-O9. Controlled Hydrothermal Synthesis of CoS₂ Microspheres toward Multifunctional Energy and Biological Applications

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CoS₂ nanoparticles were synthesized via a simple hydrothermal method, and their structural, optical, and chemical features were thoroughly examined using XRD, UV-DRS, FTIR, FE-SEM, and EDX analyses. The XRD pattern (JCPDS-41-1471) confirmed the formation of cubic metallic cobalt pyrite (CoS₂), while UV-DRS revealed a narrow band gap of ~0.47 eV, consistent with its metallic nature. FE-SEM images demonstrated quasi-cubic nanostructures. Electrochemical evaluations (CV, LSV, GCD, and EIS) established CoS₂ as an efficient electrocatalyst for the hydrogen evolution reaction (HER), exhibiting low overpotential values, small Tafel slopes. Beyond electrocatalysis, the material displayed excellent photocatalytic activity in dye degradation under UV light, highlighting its environmental remediation potential. Furthermore, antimicrobial and antifungal assays confirmed its strong inhibitory effects against pathogenic microorganisms, underscoring its multifunctional applicability in energy conversion, environmental purification, and biomedical domains.

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**6th Workshop on New Challenges of
Bionanomaterials: Science, Technology, Application,
University of Aveiro, Portugal, July 7, 2026**

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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 (WNCBM2026) with presentations and discussions specialists in Biomaterials, Nano science and Nano technology.

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Atomic Force Microscopy Methods for Characterization of Organic and Biological Low-dimensional Structures

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

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

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

This work was developed in the scope of the Project "Piezoelectricity in 2D-materials: materials, modelling, and applications" (PIEZO2D) support from the Horizon Europe Framework Programme (HORIZON-TMA-MSCA-SE), project No.101131229, "Low-dimensional ferroelectrics for advanced electronic and biomedical applications", HORIZON-WIDERA-2023-TALENTS-01, Horizon 2020 research and innovation program under grant agreement number 101186499, Latvian Council of Science Fundamental and Applied Research LZF-2025/1-0149.

Exploring the conjugation of carbon based materials with tetrapyrrolic macrocycles: New Applications and Challenges

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Photodynamic therapy (PDT) is considered as a non-invasive treatment with less side effects when compared to conventional cancer treatments. In this therapeutic approach, the activation of molecules by visible or near infrared light irradiation in the presence of dioxygen is fundamental to generate cytotoxic reactive oxygen species (ROS), responsible for cell death. Ideally, the dyes, known as photosensitisers (PS), should have an insignificant dark toxicity and some degree of hydrophilicity.

Among the high number of PS that have been studied, a special attention has been dedicated to porphyrins, corroles and phthalocyanines due to their high singlet oxygen yield, low dark toxicity and unique optical and electronic properties. However, the poor water solubility of tetrapyrrolic macrocycles can lead to aggregation compromising their use in PDT.

To prevent aggregation, several studies have been focused on the incorporation of PS into nanomaterials such as carbon nanomaterials. The development of conjugates based on tetrapyrrolic macrocycles and carbon nanomaterials for cancer therapy is a recent topic of research, with promising results found for graphene quantum dots (GQDs).

GQDs possess excellent optical and electronic properties coupled with high photostability, aqueous solubility and biocompatibility. The carboxyl and hydroxyl groups on their surface and edges enable covalent attachment, electrostatic interactions and hydrogen bonding with other suitable moieties. In the present study GQDs have been conjugated covalently and non-covalently with tetrapyrrolic macrocycles. The optical and structural characterization of the resultant hybrid materials is discussed. Preliminary studies on cellular uptake and distribution, using confocal and multiphoton microscopy, are presented.

Centre for Mechanical Technology Automation (TEMA)

Department of Mechanical Engineering, University of Aveiro

The Centre for Mechanical Technology and Automation (TEMA) is a Research and Development Unit established in 1996 and hosted by the Department of Mechanical Engineering at the University of Aveiro (Portugal). Its mission is to promote scientific and technological research of excellence, aligned with the needs of society and the industrial sector.

With a strong focus on industrial competitiveness, TEMA develops innovative solutions for manufacturing and process industries, contributing to the digital and sustainable transition. While rooted in mechanical engineering, it also invests in emerging fields such as nanotechnology, biotechnology, and artificial intelligence, reinforcing its multidisciplinary profile.

TEMA is part of the Portuguese Roadmap of Strategic Research Infrastructures and a founding member of the Associated Laboratory LASI (since 2021), where it leads the research line on Innovative and Sustainable Industries.

In 2025, TEMA was evaluated by the Fundação para a Ciência e a Tecnologia (FCT) and awarded the classification of EXCELLENT, ranking first among research units in mechanical and industrial engineering.

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- To foster collaboration with industry and society, addressing challenges in industrial transformation, climate resilience, and social impact.
- To empower researchers and partners to tackle global challenges and contribute to sustainable technological progress.

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- MP2 – Technologies for Well-being: multiscale technologies and devices for medicine, environment and energy, and smart city solutions;
- MP3 – Research Infrastructures, with and for Society: open access to laboratories and equipment, supported by technological services, consultancy, and co-creation initiatives.

This structure strengthens the link between research and industrial application, supporting technology transfer and the development of innovative solutions for sustainable industry.



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

Recovery and Resilience Plan (PRR), Portugal

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

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The greatest challenge facing humanity today is the urgent need to reduce greenhouse gas emissions in a global effort to limit the global rise in the planet's average temperatures, thereby addressing international goals of achieving carbon neutrality. In this crucial aspect, it is now perceived that the buildings in which we live, work, buy, and socialize are today responsible for about 40% of CO₂ emissions.

The ILLIANCE Agenda addresses carbon neutrality associated with the buildings sector, through the design, development, and industrialization of complementary technologies, associated with 3 fundamental pillars, namely: health, comfort and sustainability. <https://www.illiance.pt/>

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Notes

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