PRR Plano de Recuperação e Resiliência
REPÚBLICA PORTUGUESA
Financiado pela União Europeia NextGenerationEU

7th International Conference on Nanomaterials Science and Mechanical Engineering

University of Aveiro, Portugal

July 8-11, 2025

Book of Abstracts

dem
universidade de aveiro
department of mechanical engineering

tema
centre for mechanical
technology and automation

NoR CEL Network of Researchers on the Chemical Emergence of Life
Emergence ▸▸ Evolution ▸▸ Extinction
Instituto de Ciencias Nucleares UNAM
NMS&E
FIZRI Faculty of Physics University of Rijeka
LA GRANJA REVISTA CIENCIAS DE LA VIDA
DE GRUYTER OPEN CHEMISTRY Peer-reviewed open access journal
POWERI
chemosensors an Open Access Journal by MDPI
NTRIA
nmsme.org
ICNMSME

PRR Plano de Recuperação e Resiliência
REPÚBLICA PORTUGUESA
Financiado pela União Europeia NextGenerationEU

7th International Conference on Nanomaterials Science and Mechanical Engineering

University of Aveiro, Portugal

July 8-11, 2025

Book of Abstracts

dem
universidade de aveiro
department of mechanical engineering

tema
centre for mechanical
technology and automation

Title
7th International Conference on Nanomaterials Science and Mechanical Engineering
Book of Abstracts

Editors
Igor Bdikin
Gil Alberto Batista Gonçalves
Martina Kocijan

Publisher
Universidade de Aveiro

1st edition – July 2025

ISBN
978-989-9253-17-9

DOI
https://doi.org/10.48528/f7qf-yc32

This Conference has the support of “Agenda ILLIANCE [C644919832-00000035 | Project nº 46]”, “AM2R-Agenda Mobilizadora para a inovação empresarial do setor das Duas Rodas [C644866475-00000012| Project no. 15]” and “ATE-Aliança para a Transição Energética” [C644914747-00000023| Project nº nº 56]” financed by PRR – Plano de Recuperação e Resiliência under the Next Generation EU from the European Union.

Table of contents

7th International Conference on Nanomaterials Science and Mechanical Engineering

University of Aveiro, Portugal

July 8-11, 2025

(7th ICNMSME-2025)

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.

The Organizing Committee ICNMSME2025:

Prof. Dr. Robertt Valente, University of Aveiro, Portugal
Prof. Dr. Vítor António Ferreira da Costa, University of Aveiro, Portugal
Prof. Dr. António Manuel de Bastos Pereira, University of Aveiro, Portugal
Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques, University of Aveiro, Portugal
Prof. Dr. Duncan Paul Fagg, University of Aveiro, Portugal
Dr. Igor Bdikin, University of Aveiro, Portugal
Dr. Gil Alberto Batista Gonçalves, University of Aveiro, Portugal
Dr. Natália Barroca, University of Aveiro, Portugal
Dr. Francisco Loureiro, University of Aveiro, Portugal
Dr. Laura Holz, University of Aveiro, Portugal
Dr. Vanessa Cristina Diniz da Graça, University of Aveiro, Portugal

Committees

Organizing committee:

Prof. Dr. Robertt Valente
University of Aveiro, Portugal, Email: robertt@ua.pt
Prof. Dr. Vítor António Ferreira da Costa
University of Aveiro, Portugal, Email: v.costa@ua.pt
Prof. Dr. António Manuel de Bastos Pereira
University of Aveiro, Portugal, Email: abastos@ua.pt
Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques
University of Aveiro, Portugal, Email: paulam@ua.pt
Dr. Duncan Paul Fagg
University of Aveiro, Portugal, Email: duncan@ua.pt
Dr. Igor Bdikin
University of Aveiro, Portugal, Email: bdikin@ua.pt
Dr. Gil Alberto Batista Gonçalves
University of Aveiro, Email: ggoncalves@ua.pt
Dr. Natália Barroca, University of Aveiro, Portugal
University of Aveiro, Email:
Dr. Francisco Loureiro, University of Aveiro, Portugal
University of Aveiro, Email: francisco.loureiro@ua.pt
Dr. Laura Holz, University of Aveiro, Portugal
University of Aveiro, Email: lauraholz@ua.pt
Dr. Vanessa Cristina Diniz da Graça, University of Aveiro, Portugal
University of Aveiro, Email: vanessagraca@ua.pt

International organizing committee:

Dr. Vikram Uttam Pandit, Haribhai V. Desai Arts, Science & Commerce College, Pune, India
Dr. Alejandro Heredia Barbero, Universidad Nacional Autónoma de México, Mexico
Dr. Serbülent Türk, Sakarya University, Turkey
Prof. Dr. Aleksandr Bagmut, National Technical University “KhPI”, Kharkiv, Ukraine
Prof. Dr. Budhendra Kumar Singh, Central University of South Bihar, India
Prof. Dr. Robert Pullar, Università Ca’ Foscari Venezia, Italy
Prof. Dr. Natalia Tintaru, Vilnius University, Vilnius, Lithuania; Institute of Applied Physics, Chisinau, Moldova
Prof. Dr. Anderson Rodrigues Lima Caires, Federal University of Mato Grosso Do Sul, Brazil
Prof. Dr. Ajay Lad, Sant Gadge Baba Amravati University, Amravati, India

Programme committee:

Prof. Dr. Ajay Lad, Sant Gadge Baba Amravati University, Amravati, India
Dr. Alaa Almansoori, Technical Institute of Basra, Southern Technical University, Iraq
Dr. Alejandro Heredia Barbero, Universidad Nacional Autónoma de México, Mexico
Prof. Dr. Aleksandr Bagmut, National Technical University “KhPI”, Kharkiv, Ukraine
Dr. Aliaksandr Shaula, University of Aveiro, Portugal
Prof. Dr. Allisson Saiter-Fourcin, University of Normandy, Rouen, France
Dr. Ana Horovistiz, University of Aveiro, Portugal
Dr. Ana Violeta Girão, University of Aveiro, Portugal
Prof. Dr. Anderson Rodrigues Lima Caires, Federal University of Mato Grosso Do Sul, Brazil
Dr. Andrei Kovalevsky, University of Aveiro, Portugal
Prof. Dr. António Manuel de Bastos Pereira, University of Aveiro, Portugal
Dr. Anuraag Gaddam, University of Aveiro, Portugal
Dr. Bilal Fettah, Hassiba Benbouali University of Chlef, Algeria
Prof. Dr. Binay Kumar, University of Delhi, India
Prof. Dr. Budhendra Kumar Singh, Central University of South Bihar, India
Prof. Dr. Chunjiu Tang, Changshu Institute of Technology, China
Prof. Dr. Cicero R. Cena, Instituto de Física, Mato Grosso do Sul Federal University, Brazil
Dr. D. Pukazhselvan, University of Aveiro, Portugal
Dr. Dina I. Bakranova, Kazakh-British Technical University, Kazakhstan
Prof. Dr. Duncan Paul Fagg, University of Aveiro, Portugal
Prof. Dr. Erlong Wang, Northwest A&F University, Yangling, China
Prof. Dr. Eudes Borges de Araujo, Sao Paulo State University (UNESP), Brazil
Dr. Francisco Loureiro, University of Aveiro, Portugal
Prof. Dr. Georgina Miranda, University of Aveiro, Portugal
Dr. Gil Alberto Batista Gonçalves, University of Aveiro, Portugal
Dr. Gonzalo Guillermo Otero Irurueta, University of Aveiro, Portugal
Prof. Dr. Gunnar Suchaneck, Technische Universität Dresden, Germany
Prof. Dr. Henrikas Cesiulis, Vilnius University, Lithuania
Dr. Igor Bdikin, University of Aveiro, Portugal
Dr. Indrani Coondoo, University of Aveiro, Portugal
Dr. Isabel Duarte, University of Aveiro, Portugal
Dr. Joana Catarina Mendes, University of Aveiro, Portugal
Dr. Joana Mesquita-Guimaraes, University of Aveiro, Portugal
Dr. João Miguel Serras Dias, University of Aveiro, Portugal
Dr. Laura Holz, University of Aveiro, Portugal
Prof. Dr. Marcos Gomes Ghislandi, Universidade Federal Rural de Pernambuco, Brazil
Dr. Martina Kocijan, University of Zagreb, Croatia
Dr. Milan Vukšić, Jožef Stefan Institute, Ljubljana, Slovenia
Prof. Dr. Musaab ZAROG, Sultan Qaboos University, Oman
Dr. Natália Barroca, University of Aveiro, Portugal
Prof. Dr. Natalia Tintaru, Vilnius University, Vilnius, Lithuania; Institute of Applied Physics, Chisinau, Moldova
Prof. Dr. Neeraj Panwar, Central University of Rajasthan, Bandarsindri, India
Dr. Oleksandr Tkach, University of Aveiro, Portugal
Prof. Dr. Radheshyam Rai, Eternal University, India
Prof. Dr. Reinhard Schwarz, Instituto Superior Técnico, Lisboa, Portugal

Dr. Ricardo Beja, University of Aveiro, Portugal
Prof. Dr. Robert Pullar, Università Ca' Foscari Venezia, Italy
Dr. Pankaj Bharmoria, Barcelona Materials Science Institute (ICMAB-CSIC), Barcelona, Spain
Dr. Pavani Krishnapuram, University of Aveiro, Aveiro, Portugal
Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques, University of Aveiro, Portugal
Dr. Pavel Zelenovskii, University of Aveiro, Portugal
Prof. Dr. Salam J.J. Titinchi, University of the Western Cape, Cape Town, South Africa
Prof. Dr. Senentxu Lanceros-Méndez, Parque Científico y Tecnológico de Bizkaia, Spain
Dr. Serbülent Türk, Sakarya University, Turkey
Dr. Suresh Kumar Jakka, University of Aveiro, Portugal
Dr. Svitlana Kopyl, University of Aveiro, Portugal
Dr. Venkata Ramana Eskilla, University of Aveiro, Portugal
Dr. Vikram Uttam Pandit, Haribhai V. Desai Arts, Science & Commerce College, Pune, India
Prof. Dr. Vítor António Ferreira da Costa, University of Aveiro, Portugal
Dr. Zhi Jiang, University of Aveiro, Portugal

Editorial Board:

Dr. Igor Bdikin, University of Aveiro, Portugal
Dr. Gil Alberto Batista Gonçalves, University of Aveiro, Portugal
Dr. Martina Kocijan, University of Zagreb, Croatia

Technical Program Committee:

Prof. Dr. Duncan Paul Fagg, University of Aveiro, Portugal
Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques, University of Aveiro, Portugal
Dr. Igor Bdikin, University of Aveiro, Portugal
Dr. Gil Alberto Batista, University of Aveiro, Portugal
Dr. Francisco Loureiro, University of Aveiro, Portugal
Dr. Natália Barroca, University of Aveiro, Portugal
Dr. Laura Holz, University of Aveiro, Portugal
Dr. Vanessa Cristina Diniz da Graça, University of Aveiro, Portugal
Dr. Ricardo Beja, University of Aveiro, Portugal
Dr. Indrani Coondoo, University of Aveiro, Portugal
Dr. Joana Mesquita-Guimaraes, University of Aveiro, Portugal
Dr. Pavel Zelenovskii, University of Aveiro, Portugal
Dr. Zhi Jiang, University of Aveiro, Portugal
Mr. Luís César da Silva Ribeiro, University of Aveiro, Portugal
Ms. Dina Teresa Marques da Silva, University of Aveiro, Portugal
Ms. Maria José Haneman Marques, University of Aveiro, Portugal

Conference Contacts:

TEMA-ICNMSME-2025.aveiro@ua.pt

Telefone: +351 234 370 830

Conference Web:

https://icnmsme2025.web.ua.pt/

ICNMSME2025 program

July 8, 2025 (Tuesday)

7th International Conference on Nanomaterials Science and Mechanical Engineering (7th ICNMSME-2025)	
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	CHAIRS: Dr. Natália Barroca , Dr. André Girão Session: **New Materials and Advanced Materials** ***Keynote talk*** Dr. Gil Gonçalves **(I9)** **Carbon Dots Driving Innovation in Health and Environmental Technologies** *Centre for Mechanical Technology and Automation (TEMA), Mechanical Engineering Department, University of Aveiro, 3810-193 Aveiro, Portugal*
9:30- 10:00	Session: **Biomaterials** ***Plenary Lecture*** Prof. Dr Ana Marina Ferreira Duarte **Biomimetic hydrogels and engineering strategies for functional tissue regeneration** *School of Engineering, Newcastle University, Newcastle-Upon-Tyne, UK*
10:00- 10:10	Coffee break
10:10- 10:30	Session: **Biomaterials** ***Keynote talk*** Dr. Priscila Melo **(I21)** **Tuneable, Printable, Injectable: Next-Gen Hydrogels for Functional Tissue Reconstruction** *School of Engineering, Newcastle University. Newcastle Upon Tyne, United Kingdom*

10:30- 10:45	Session: **Biomaterials** Dr. Merve KEYF **(O33)** **Effect of LiCl and CaCl2 Concentration on Physicochemical Properties of Sodium Alginate- Based Hydrogel** *Sakarya University, Biomedical Engineering, Institute of Natural Sciences, Esentepe Campus, 54187, Sakarya, Turkey*
10:45- 11:10	Session: **Biomaterials / New Energy Materials** ***Keynote talk*** Dr. Pavel Zelenovskii **(I5)** **Supramolecular one- and two-dimensional peptide nanostructures for energy storage and harvesting** *Department of Physics and CICECO, University of Aveiro, 3810-193 Aveiro, Portugal*
11:10- 11:25	Session: **Biomaterials** Muhammet Kamil Kerim **(O15)** **Innovative Multifunctional Hydrogel Dressings with Natural Antimicrobial Extracts for Enhanced Diabetic Wound Healing** *Sakarya University, Institute of Natural Sciences, Department of Biomedical Engineering, 54187, Sakarya, Turkiye*
11:25- 11:40	Session: **Biomaterials** Selen Şakar **(O16)** **Synthesis, swelling behavior and water retention capacity of self-healing gelatin-chitosan-silk sericin hydrogels** *Sakarya University, Institute of Natural Sciences, Department of Chemistry, 54187, Sakarya, Turkiye*
11:40- 12:00	Session: **Polymer Composites** ***Keynote talk*** Dr. Indrani Coondoo **(I12)** **Multifunctional PVDF-based polymer composites: opportunities in energy applications** *University of Aveiro, Aveiro 3810-193, Portugal*
12:00- 12:15	Session: **Biomaterials** Dr. David Adeyemi **(O20)** **Green synthesis of silver nanoparticles of Spondias Mombin and Terminalia Ivorensis ethanolic extracts and investigation of their antimicrobial activities** *Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Lagos, Nigeria*
12:15- 12:30	Session: **Biocompatible nanomaterials** ***Keynote talk*** Prof. Dr. Sammia Shahid **(O8)** **Therapeutic Assessment of Antidiabetic Efficiency of Co3O4 and TiO2 Nanoparticles on alloxan-induced diabetic mice: An Experimental Study** *Department of Chemistry, School of Science, University of Management and Technology Lahore-54770 Pakistan*

12:30-14:00	Lunch
14:00-14:30	CHAIRS: Dr. Pavel Zelenovskii, Dr. Indrani Coondoo Session: **Nanotechnology** ***Plenary Lecture*** Prof. Dr Senentxu Lanceros-Méndez **Optimizing response of printable magnetorheological elastomers for advanced applications** *BCMaterials, UPV/EHU Science Park, Leioa, Spain* *Ikerbasque, Basque Foundation for Science, Bilbao, Spain* *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*
14:30-14:50	Session: **Low Dimension Structures** ***Keynote talk*** Prof. Dr. Yuri Pusep **(O5)** **Current-induced Light Emission in Mesoscopic Electron-hole Plasma** *São Carlos Institute of Physics, University of São Paulo, 13560-970 São Carlos, SP, Brazil*
14:50-15:10	Session: **Hydrogen and Fuel Cell Science** ***Keynote talk*** Dr. Francisco J. A. Loureiro **(I15)** **Layered cobaltite electrodes for Protonic Ceramic Cells** *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*
15:10-15:30	Session: **Nanocomposites** ***Keynote talk*** Prof. Dr. Vikram Uttam Pandit **(I1)** **Recent Advancements in Photocatalysis Using Nanocomposites** *Haribhai V. Desai College of Arts, Science and Commerce (Autonomous) Pune, India*
15:30-15:45	Coffee break
15:45-16:05	Session: **Biomaterials** ***Keynote talk*** Dr. Natália Barroca **(I26)** **Exploiting strain gradients in biomaterials to conceptualize advanced bone grafts** *Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Aveiro, Portugal*

16:05- 16:25	Session: **Sensor Materials** ***Keynote talk*** Prof. Dr. Andrzej Kudelski **(I3)** **Comparison of functionality and sensitivity of surface-enhanced Raman scattering and surface plasmon resonance sensors for DNA identification: Identification of BRCA1 gene mutation variants in clinical samples** *Faculty of Chemistry, University of Warsaw, Poland*
16:25- 16:45	Session: **Photocatalysis** ***Keynote talk*** Dr. Matejka Podlogar **(I10)** **ZnO Nanorods as Photocatalysts for the Degradation of Organic Pollutants in Water** *Jožef Stefan Institute, Ljubljana, Slovenia*
16:45- 17:05	Session: **Nanotechnology** ***Keynote talk*** Prof. Dr. Serbülent Türk **(I4)** **Contact Angle Measurement with Simplified Approach and Applications** *Sakarya University, Biomedical, Magnetic and Semiconductor Materials Research Center (BIMAS-RC), 54187, Sakarya, Turkey*
17:05- 17:25	Session: **Hydrogen Storage** ***Keynote talk*** Dr. D. Pukazhselvan **(I28)** **Modern Approaches of Energy Storage through Magnesium Hydride for Vehicular Applications** *Department of Mechanical Engineering, TEMA - Centre for Mechanical Technology and Automation, University of Aveiro, Aveiro 3810-193, Portugal* *LASI - Intelligent Systems Associate Laboratory, Guimarães 4800-058, Portuga*
17:25- 17:45	Session: **Optical Materials** ***Keynote talk*** Dr. Suresh Kumar Jakka (I24) **Rare earth doped low phonon glasses for gas sensing** *i3N and Department of Physics, University of Aveiro, Aveiro, 3810-193, Portugal*
17:45- 18:00	Session: **Environmental Friendly Materials** Prof. Dr. Sirajo Abubakar Zauro **(O12)** **Acacia gum-graft Copolymer Hydrogel: Preparation and Metal ions Adsorption studies** *Department of Energy and Applied Chemistry, Usmanu Danfodiyo University, Sokoto, PMB 2346, Sokoto, Nigeria*

July 9, 2025 (Wednesday)

7th International Conference on Nanomaterials Science and Mechanical Engineering (7th ICNMSME-2025)

8:30-8:45	CHAIRS: Dr. Andrei Kovalevsky, Dr. Anuraag Gaddam Session: **Nano-Composite** Ganesh P. Jadhav **(O1)** **Synthesis, Characterization of Pr(OH)3 -PQ Nano-Composite for Enhanced Photocatalytic Activities** *Haribhai V. Desai College of Arts, Science and Commerce (Autonomous) Pune, India*
8:45-9:00	Session: **Biomaterials** Mohmad ABOBAKER **(O37)** **Preparation and Characterization of Smart Hydrogel Drug Delivery System** *Biomedical Engineering, Institute of Natural Sciences, Sakarya University, Esentepe Campus, 54187 Sakarya, Türkiye*
9:00-9:20	Session: **Nanotechnology, Sensor Materials** ***Keynote talk*** Prof. Dr. Sultan Ben Jaber **(I8)** **High sensitive setup of gold nanorods substrates for explosives detection using surface enhanced Raman spectroscopy** *Forensic Chemistry, Department of Forensic Science, King Fahad Security College, Riyadh 13232, Saudi Arabia*
9:20-9:35	Session: **Thin films** ***Keynote talk*** Dr. Martina Kocijan **(I14)** **A comparison of thermal and plasma-enhanced atomic layer deposition techniques of TiO2 thin films for the photocatalytic degradation of pollutants from water** *Faculty of Physics, University of Rijeka, Radmile Matejčić 2, 51 000 Rijeka, Croatia*
9:35-10:00	Session: **Manufacturing Waste Management and Waste Disposal** ***Keynote talk*** Prof. Dr. Natalia Tsyntsaru **(I6)** **Routes for Eco-Friendly Recovery of Palladium and Platinum** *Faculty of Chemistry and Geosciences, Vilnius University, 03225 Vilnius, Lithuania* *Institute of Applied Physics, Moldova State University, 2028 Chisinau, Moldova*
10:00-10:20	Coffee break

10:20-11:00	Session: **Magnetic Materials** ***Plenary Lecture*** Prof. Dr. Robert C. Pullar **Magnetic metallic nanoparticles produced from oxide precursors via pyrolysis without the use of added reducing agents or a reductive atmosphere** *Dipartimento di Scienze Molecolari e Nanosistemi (DSMN), Università Ca' Foscari Venezia, Venezia Mestre, Venezia (VE) 30172, Italy*
11:00-11:30	Session: **Neuromorphic Technologies** ***Plenary Lecture*** Prof. Dr. Nikolai A. Sobolev **Material-related problems of neuromorphic technologies** *Departamento de Física & i3N, Universidade de Aveiro, 3810-193 Aveiro, Portugal*
11:30-12:00	Session: **Magnetic Materials** ***Plenary Lecture*** Prof. Dr. Gunnar Suchaneck **Estimation of the degree of antisite disordering of magnetoactive ions in Sr2FeMoO6-δ by means of the intensity of the X-ray peak (101)** *TU Dresden, Institute for Solid-State Electronics, 01062 Dresden, Germany*
12:00-12:20	Session: **Nanotechnology** Prof. Dr. Burak ÜNLÜ **(O22)** **Zeta Potential and Particle Size Investigation on Bentonite Activation** *Sakarya University, Biomedical, Magnetic and Semiconductor Materials Research Center (BIMAS-RC), 54187, Sakarya, Turkey*
12:20-12:40	Session: **Hydrogen and Fuel Cell Science** ***Keynote talk*** Dr. Laura Holz **(I29)** **Exploring transition metal nitrides as anode for ammonia solid oxide fuel cells** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal* *LASI - Intelligent Systems Associate Laboratory, Portugal*
12:40-14:00	Lunch
14:00-14:40	Session: **Electrochemical sensors** CHAIRS: Dr. Pavani Krishnapuram, Dr. Martina Kocijan ***Plenary Lecture*** Prof. Dr. Ajeet Kaushik **Point-of-care Electrochemical Sensing of Microplastic for Environmental Surveillance** *Department of Civil and Environmental Engineering, Florida Polytechnic University, Lakeland, Florida-USA*

14:40- 15:20	Session: **Biotechnology** ***Plenary Lecture*** Prof. Dr. Philip Leduc **What is up with Nature? One Mechanical Engineer’s View** *Departments of Mechanical Engineering, Biomedical Engineering, Computational Biology, and Biological Sciences, Carnegie Mellon University, USA*
15:20- 15:40	Session: **Intelligent Manufacturing** ***Keynote talk*** Prof. Dr. Musaab ZAROG **(I17)** **Artificial Intelligence (AI) Applications in Manufacturing** *Department of Mechanical and Industrial Engineering, College of Engineering, Sultan Qaboos University, P.O. Box 33, Al-Khoudh, Muscat, 123, Sultanate of Oman*
15:40- 16:10	Session: **Ceramics** ***Keynote talk*** Prof. Dr. Andrei V. Kovalevsky **(I2)** **Engineering ceramic thermoelectrics: from design to functional performance** *CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Portugal*
16:10- 16:25	Session: **Ceramics** Miguel Vieira **(O24)** **Design of SrTiO3-Based Thermoelectric Composites with In Situ Exsolved Mo–Ni Alloys for Enhanced Performance** *CICECO – Aveiro Institute of Materials, Department of Materials Engineering and Ceramics (DEMaC), University of Aveiro, 3810-193, Aveiro, Portugal*
16:25 16:50	Coffee break
16:50 18:00	**Poster Session (P1-P21)**
20:00 21:30	**Conference Banquet**

July 10, 2025 (Thursday)

Auditorium 1 **2nd Workshop on High Valued Developments in Photocatalysis**		**Auditorium 2** **7th International Conference on Nanomaterials Science and Mechanical Engineering (7th ICNMSME-2025)**	
9:00–9:05	**Dr. Vikram Pandit** Introduction to Workshop	9:00–9:20	CHAIRS: Dr. Laura Holz, Dr. Gil Gonçalves Session: **New Materials and Advanced Materials** Dang Lam Tuan Cuong **(O2)** **Developing 3D Aerogel from Magnetized Graphene Oxide and Biomass-derived Cellulose for Effective Antibiotics Removal** *Laboratory of Advanced Materials Chemistry, Institute for Advanced Study in Technology, Ton Duc Thang University, Ho Chi Minh City, Vietnam*
9:05–9:10	**Dr. Igor Bdikin** Welcome on behalf of Conference		
9:10-9:15	**Dr. Rajendra Gurao** Principal, Welcome of all participants		
9:15–9:40	***Keynote talk*** **Dr. Vivekanand Jawale** Topic: Dual-Functional Zinc Oxide Nanostructures: Harnessing Environmental Remediation and Antioxidant Potential through Ag-Embedded Composites	9:20–9:40	Session: **Nanotechnology** Prof. Dr. Erlong Wang **(O38)** **Nanotechnology and nanocarrier vaccine in aquaculture** *College of Animal Science and Technology, Northwest A&F University, Yangling, Shaanxi 712100, China*
9:40 – 9:50	**Dawange Ganesh Punjaba** Green synthesis of copper oxide nanocatalyst using plant extract and its antibacterial and photocatalytic applications	9:40–10:00	Session: **Multifunctional Nanomaterials** ***Keynote talk*** Prof. Dr. Neeraj Panwar **(I16)** **Exploring Multifunctionality: Optical, Impedance, and Photocatalytic Properties of Dy0.5Er0.5CrO3 Nanomaterial** *Department of Physics, Chaudhary Charan Singh University Meerut-250004, Uttar Pradesh, India*

9:50 - 10:00	**Beg Waseem Ahamad** A Colorimetric Detection Probe for Al(III) by phenolphthalein hydrazone Schiff Base	10:00– 10:20	Session: **Ceramics** ***Keynote talk*** Prof. Dr. Radheshyam Rai **(I25)** **Ellipsometric study of {Pb(Mg1/3Nb2/3)O3}1-x {PbTiO3}x: Evaluation of refractive index, extinction coefficient and optical band gap** *School of Basic and applied sciences, Department of Physics, Galgotias University Greater Noida, Gautam Buddh Nagar, Uttar Pradesh-203201 India*
10:00- 10:10	**Tushar Mahadev Patil** Graphitic Carbon Nitride: Effect of various precursors on dye degradation and drug degradation		
10:10– 10:20	**Ms. Rohini Baban Thakare** Recent Advances in the Synthesis and Characterization of Schiff Base Ligands and Their Metal Complexes: A Pathway to Functional Materials		
10:20– 10:40	Coffee break / Open discussions		
10:40– 10:50	**Thombare Sakshi Shamrao** 6,13-Pentacenequinone and 5, 7, 12, 14-Pentacenetetrone for Photocatalytic Applications	10:40– 11:00	Session: **Micro / Nano Materials** ***Keynote talk*** Prof. Dr. Marcos G. Ghislandi **(I19)** **Portable desalinator using graphene oxide functionalized microporous membranes** *Engineering Campus (UACSA), Federal Rural University of Pernambuco (UFRPE), 54518-430 Cabo de Santo Agostinho, PE, Brazil*
10:50– 11:00	**Purnima Mallikarjun Patil** Enhanced Photocatalytic Degradation of Methylene blue using SnO 2- PQ nanocomposite		
11:00– 11:10	**Bhagwan Daphal** Polyaniline: Robust Green Light-Driven Photocatalyst for Multi-Textile Dye Degradation	11:00– 11:15	Session: **New Materials and Advanced Materials** Oumayma BOUHAJEB **(O13)** **TiO2/SiO2/MAPbCl3 photocatalyst for tartrazine removal: Synthesis, characterization and reusability** *Laboratoire de Chimie Minérale Appliquée (LCMA) LR19ES02, Faculté des Sciences de Tunis, Université Tunis El Manar. Campus Universitaire Farhat HACHED, 2092, El Manar – Tunis, Tunisie*

11:10–11:20	**Mithari Jatin** AbhayPentacenequinone/BiOI (BiOX, X = I) Photocatalyst for Dye Degradation	11:15–11:30	Session: **Composites** Oumayma BOUHAJEB **(O14)** **Mn doping MAPbCl3/TiO2/SiO2: A promising strategy for less lead perovskite based photocatalyst toward tartrazine degradation** *Laboratoire de Chimie Minérale Appliquée (LCMA) LR19ES02, Faculté des Sciences de Tunis, Université Tunis El Manar. Campus Universitaire Farhat HACHED, 2092, El Manar – Tunis, Tunisie* *Sakarya University, Biomaterials, Energy, Photocatalysis, Enzyme Technology, Nano & Advanced Materials, Additive Manufacturing, Environmental Applications and Sustainability Research & Development Group (BIOENAMS R&D Group), 54050 Sakarya, Turkiye*
11:20–11:30	**Ganesh Jadhav** Synthesis, Characterization of Pr(OH)3 Nanowires for Enhanced Photocatalytic Activities		
11:30–11:40	**Kavita Mahaveer Durgade** Synthesis and Characterization of nitrogen containing heterocyclic Quinazoline Derivatives	11:30–11:45	Session: **Engineering Optimization** Sasidhar Pentapati **(O18)** **Manufacturing and Optimization of the properties of Jute-Kevlar/Nano Fumed Silica hybrid reinforced epoxy composite using Taguchi technique** *School of Mechanical Sciences, Indian Institute of Technology Bhubaneswar, Odisha, India*
11:40–11:50	**Bhalerao Priyanka Ganesh** Synthesis and characterisation of transition metal sulphide nanoparticles as an efficient photo & electrocatalyst for efficient Hydrogen evolution		
12:00–14:00	**Lunch**		

4th International Workshop on "Modern Trends in Energy Research" WMTER-2025		7th International Conference on Nanomaterials Science and Mechanical Engineering (7th ICNMSME-2025)	
14:00–14:05	Workshop introduction and welcome Address D. Pukazhselvan (Convener WMTER 2025)	**14:00–14:20**	CHAIRS: Dr. Suresh Kumar Jakka Session: **Photocatalytic Materials** Sakshi Thombare **(O23)** **Metal loaded 6,13-Pentacenequinone and 5, 7, 12, 14-Pentacenetetrone for Photocatalytic Applications** *Department of Chemistry, PES's Modern College of Arts, Science & Commerce, Pune-05, India* *Haribhai V. Desai College, Pune-02, India*
14:05–14:40	**Session:1** **Chair: Francisco Loureiro** **(Co-convener, WMTER 2025)** **Plenary Lecture** **Fausthon Fred da Silva** Department of Chemistry, Federal University of Paraíba, Brazil ***Title: "Phyto-mediated green synthesis of NiO nanoparticles for OER electrocatalysis"***	**14:20–14:35**	Session: **Biomaterials** Dilek BAYRAKDAR **(O36)** Development and Characterization of PEG-CMC-CNT Containing Hydrogels for Drug Delivery Systems *Biomedical Engineering,* *Institute of Natural Sciences, Sakarya University, Esentepe Campus, 54187 Sakarya, Türkiye*
14:40–15:00	**Keynote Address** **Ihsan Çaha** International Iberian Nanotechnology Laboratory, Braga, Portugal ***Title: "Ultrafast Transmission Electron Microscopy: A New Frontier for Dynamic Imaging at the Nanoscale"***	**14:35–14:50**	Session: **Photocatalysis** Ganesh Dawange **(O19)** **Green synthesis of copper oxide nanocatalyst using plant extract and its antibacterial and photocatalytic applications** *Haribhai V. Desai College, Pune, India* *Sanjivani College of Engineering, Kopargaon, India*

15:00– 15:20	**Session:2** **Chair: Vanessa Graca** **Invited Talk-1** **Allan J. M. Araújo** TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal ***Title: “Layered Ruddlesden–Popper lanthanum nickelates for SOC oxygen electrodes: Effect of PrOx impregnation”***	**14:50– 15:05**	Session: **Micro / Nano Materials** Prof. Dr. Jamal Davoodi **(O3)** **Molecular dynamics simulation of Titanium Carbide MXene/Graphene heterostructure** *Department of Physics, Faculty of science, University of Zanjan, Zanjan, Iran*
		15.05– 15.20	Session: **Biomaterials/Surface Engineering** Rabia Güzide **(O32)** **New Type Aortic Valve Design: Enhancing Surface Properties with Biofunctional Polymer Coatings** **Green synthesis of silver nanoparticles of Spondias Mombin and Terminalia Ivorensis ethanolic extracts and investigation of their antimicrobial activities** *Biomedical Engineering, Institute of Natural Sciences, Sakarya University, Esentepe Campus, 54187 Sakarya, Türkiye*
15.20– 15.40	**Invited Talk-2** **Paula Rosendo Santos** Facultad de Farmacia, Departamento de Química y Bioquímica, Urbanización Montepríncipe, Universidad San Pablo-CEU, CEU Universities, E-28668 Madrid, Spain ***Title: “Unveiling the Mechanism of Exsolution of Silver Nanoparticles for Decorating Lanthanum Strontium Ferrite and assessment of its electrochemical behavior”***	**15.20– 15.35**	Session: **Optical materials** Raphael de S. Flores **(O29)** **Synthesis, characterization, and evaluation of cellulose acetate nanoparticles as a photosensitizing agent in photodynamic inactivation against S. aureus and E. coli bacteria** *Instituto de Física – Universidade Federal de Mato Grosso do Sul, Brazil*

15.40–16.00	**Invited Talk-3** **Jayakrishnan K. Ravindran** TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal ***Title: "Environmental Assessment of MSW-to-FT Fuel Pathways: Impact of Gasification and Tail Gas Utilization Strategies"***	**15.35–15.50**	Session: **Micro / Nano Materials** Dr. Regiane Godoy de Lima **(O27)** **Determination of Photosensitizing Potential of Lapachol for Photodynamic Inactivation of Bacteria** *Optics and Photonics Group, Institute of Physics, Federal University of Mato Grosso do Sul, P.O. Box 549, 79070-900 Campo Grande, MS, Brazil*
16.00–16.20	**Invited Talk-4** **Carlos O Amorim** Department of Physics and i3N, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal ***Title: "Low-Temperature, Rapid Synthesis of Cu3BiS3 Thin Films for Sustainable Photovoltaics"***	**15.50–16.05**	Session: **Micro / Nano Materials** Maria Victória Pereira Dias **(O26)** **Synthesis and Characterization of Polymer Nanoparticles Loaded with Lapachol for Biomedical Applications** *Optics and Photonics Group, Institute of Physics, Federal University of Mato Grosso do Sul, P.O. Box 549, 79070-900 Campo Grande, MS, Brazil*
16.20–16.30	**Coffee break / Open discussions**		
16:40–17:00	**Session:2** **Chair: Laura Holz** **Invited Talk-5** **Jaykumar Lachure** Department of Computer Engineering & Information Technology, VJTI Mumbai, India ***Title: "Quantum-Informed Generative Optimization (QIGO) for Catalyst-Free Hydrogen Evolution Using Hybrid Quantum-AI"***	**16:20–16:35**	Session: **Micro / Nano Materials** Emmanuel S.C. Miguel **(O25)** **Nanoplastics Fragmentation and Characterization Using a Solvent-Free Method** *Institute of Physics, Federal University of Mato Grosso do Sul, Av. Costa e Silva, s/nº Campo Grande, MS, Brazil*

		16:35–18:00	**Virtual Poster Session (P1-P21)**
17:00–17:20	Invited Talk-6 **Morena B. Farias** Department of Materials Science and Engineering Postgraduate Program, Federal University of Rio Grande do Norte, Brazil ***Title: "Improvement of cobalt-free perovskite electrodes for application in solid oxide fuel cells"***		
17:20–17:40	Invited Talk-7 **Raquel Dantas** Department of Chemistry, University of Aveiro, Portugal ***Title: "From Design to Performance: Redox-active COFs as advanced organic electrode materials"***		
17.40–17.55	Invited Talk-8 **D. Pukazhselvan** TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal ***Title: "Reactive Hydride Composites: A Promising Pathway for High-Capacity Hydrogen Storage"***		
17:55-18:00	**Vote of Thanks/Concluding remarks**		

July 11, 2025 (Friday)

7th International Conference on Nanomaterials Science and Mechanical Engineering (7th ICNMSME-2025)

9:00- 9:20	CHAIRS: Dr. Francisco Loureiro, Prof. Dr. Manish Jugroot Session: **Thin films** ***Keynote talk*** Dr. Oleksandr Tkach **(I11)** **Stress effect on the structure of polycrystalline potassium sodium niobate piezoelectric thin films** *CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Aveiro, Portugal*
9:20- 9:40	Session: **Nanocomposites** Dr. Vivekanand Jawale **(O30)** **Ag-Embedded Composites Ag-ZnO Nanostructures for Sustainable Solutions: Synergistic Photocatalytic Degradation and Antioxidant Efficacy** *Department of Chemistry, Modern College of Engineering Shivajinagar, Pune-411005, India*
9:40- 10:00	Session: **Micro/Nano Materials** ***Keynote talk*** Prof. Dr. Manish Jugroot **(I22)** **Porous Materials for Multimodal Micro-propulsion Systems for Small Spacecraft** *Mechanical and Aerospace Engineering, Royal Military College of Canada, Kingston, Canada*
10:00- 10:15	Coffee break
10:15- 10:30	Session: **Composites** Tushar Patil **(O28)** **Graphitic Carbon nitride: Effect of various precursors on dye degradation and drug degradation** *Dr. Yusuf Hamied Department of Chemistry, Ramnarain Ruia Autonomous College, Mumbai 400019, India*
10:30- 11:00	Session: **Biomaterials** ***Keynote talk*** Dr. Pankaj Bharmoria **(I13)** **Shifting the Action Spectrum of Azobenzene into the Red/NIR Region via Triplet-sensitization** *Institute of Materials Science of Barcelona, ICMAB-CSIC, Bellaterra, Barcelona, 08193, Spain*

11:00- 11:15	Session: **Nanotechnology** Dr. Monther Alsboul **(O35)** **Investigation of Thermal Conductivity in Ethylene Glycol-Based Nanofluids Containing Er_2O_3 and Co_3O_4 Nanoparticles** *Department, College of Science, Al Hussein Bin Talal University, Jordan*
11:15- 11:35	Session: **Hydrogen and Fuel Cell Science** ***Keynote talk*** Dr. Vanessa Graça **(I27)** **Metal-Supported Proton-Conducting Electrochemical Cells: MnO2 as a promising sintering additive** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.* *LASI - Intelligent Systems Associate Laboratory, Portugal*
11:35- 11:50	Session: **New Materials and Advanced Materials** Prof. Dr. Soner ÇAKAR **(O11)** **Effectiveness of TiO2/MoS2 nanocomposite electrodes prepared on ITO in the oxygen evolution reaction** *Zonguldak Bülent Ecevit University, Faculty of Science, Department of Chemistry, 67100 Zonguldak, Turkiye* *Sakarya University, Biomaterials, Energy, Photocatalysis, Enzyme Technology, Nano & Advanced Materials, Additive Manufacturing, Environmental Applications and Sustainability Research & Development Group (BIOENAMS R&D Group), 54050 Sakarya, Turkiye*
11:50- 12:05	Session: **New Materials and Advanced Materials** Nathalia Hammes **(O10)** **Development of Advanced Co-axial Phase Change Fibres for Thermoregulation of Civil Engineering Materials** *Centre of Physics of Minho and Porto Universities (CF-UM-UP), Campus Azurém, University of Minho, Av. da Universidade, 4800-058 Guimarães, Portugal* *Centre for Textile Science and Technology (2C2T-UMinho), Campus Azurém, University of Minho, Av. da Universidade, 4800-058 Guimarães, Portugal*
12:05- 12:20	Session: **Composites** Dr. Bilal FETTAH **(O9)** **Effect of different steel wires diameter on the reinforcement of jute/polyester resin composite** *LRM, Mechanical Engineering Department, Faculty of Technology, Hassiba Benbouali University of Chlef, P.O. Box 151, Esalem City, Chlef, 02000, Algeria*
12:20- 14:00	Lunch

14:00- 14:30	CHAIRS: Dr. Vanessa Graça, Dr. Oleksandr Tkach Session: **New Materials and Advanced Materials** ***Keynote talk*** Prof. Dr. Carlos Granadeiro **(I18)** **Valorization of cork residues as adsorbents for water treatment** *LAQV-REQUIMTE, Department of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, 4169-007 Porto, Portugal*
14:30- 14:45	Session: **Composites** Ayoub Grouli **(O21)** **Sustainable Adsorption of Congo Red Dye Using Natural Bentonite and Hydroxyapatite: Mechanistic Insights, Optimization, and Reusability** *Laboratory of Health and Biology (LBS), Faculty of Sciences Ben M'Sick, Department of Chemistry, University Hassan II of Casablanca, Casablanca, 20000, Morocco*
14:45- 15:00	Session: **Biomaterials** Mahsa Heidarnejad **(O17)** **Synthesis, Characterization, and Drug Release Profile of PEG-Coated Fe_3O_4 Magnetic Nanoparticles Loaded with Dexamethasone** *Sakarya University, Institute of Natural Sciences, Department of Chemistry, 54187 Sakarya, Turkiye*
15:00- 15:15	Session: **Protective Coatings and Corrosion of Materials** Amira GHARBI **(O6)** **Enhanced Corrosion and Wear Resistance of Nickel Coatings on Copper in NaCl Media via the Integration of Synthesized Graphene** *Laboratory of Physics of Matter and Radiation (LPMR), Faculty of Science and Technology, University Mohamed Cherif Messaadia, BP 1553-41000 Souk Ahras, Algeria*
15:15- 15:30	Session: **Environmental Friendly Materials** Teodora Vukša **(O34)** **Rheological Behavior of Natural Rubber Modified with Industrial Herbal Dust Ash** *University of Novi Sad, Faculty of Technology Novi Sad, Bulevar cara Lazara 1, 21000 Novi Sad, Serbia*
15:30- 15:45	Coffee break
15:45- 16:00	Session **Low Dimension Structures** Justyna Niewiadomska-Kaplar **(O7)** **Atomic system: reticular spatial structure as engineering model of atomic shells and the meaning of the periodic table** *Tab edizioni, viale Manzoni, 24C - 00185 Roma (RM), Italy*

16:00- 16:20	Session: **Composites** FALAH Fatima Zahra **(O4)** **Synergistic Composite Adsorbents for Advanced Radioactive Decontamination and Environmental Safety** *Laboratory of Analytical and Molecular Chemistry, Faculty of Sciences Ben M'Sick, Hassan II University of Casablanca, Morocco* *National Center of Science, Technology and Nuclear Energy (CNESTEN), Morocco; Center for Nuclear Maamoura (CENM), Rabat, Morocco*
16:20- 16:40	Session: **Optical Materials** ***Keynote talk*** Dr. Pavani Krishnapuram **(I7)** **A-site substituted Aurivillius Rare earth Perovskite structures: A pathway to tunable optoelectronic properties** *i3N & Department of Physics, University of Aveiro, Aveiro 3810-193, Portugal*
16:40- 17:00	Session: **Nanotechnology** ***Keynote talk*** Dr. Zhi Jiang **(I20)** **Vacancy diamond color centers process with machine learning** *TEMA, Mechanical Engineering Department, University of Aveiro, Aveiro, 3810-193, Portugal*
17:00- 17:20	Session: **Low Dimensions Structures** Prof. Dr. Yulian Vysochanskii **(O31)** **Raman spectroscopy study of structural transformations in van der Waals ferrielectric CuInP2S6** *Institute for Solid State Physics and Chemistry, Uzhhorod National University, Uzhhorod, Ukraine*
17:20- 17:40	Session: **Low Dimensions Structures** ***Keynote talk*** Dr. Venkata Eskilla **(I23)** **Tailoring piezoelectrics for enhanced energy storage** *I3N, Department of Physics, University of Aveiro, 3810-193, Aveiro, Portugal*
17:40- 18:00	**Conference Closing Ceremony**

Poster session, July 9, 2025 (Thursday), 16:00-18:30

P1	**Zn-MOF as an efficient catalytic platform for the conversion of waste polyethylene terephthalate bottles into bis(2-hydroxyethyl) terephthalate** Rubi Bhakhar, Rik Rani Koner *School of Chemical Sciences and Advanced Materials Research Center, Indian Institute of Technology Mandi, Kamand, Mandi 175075, Himachal Pradesh, India; School of Mechanical and Materials Engineering, Indian Institute of Technology Mandi, Kamand, Mandi 175075, Himachal Pradesh, India*
P2	**Anelastic-elastic body of nanocomposites of multiwalled carbon nanotubes and polymers, SiO2** A.P. Onanko, M.V. Yatsiuk, Y.A. Onanko, O.P. Dmytrenko, M.P. Kulish, T.M. Pinchuk-Rugal, D.V. Charnyi, E.M. Matselyuk, O.L. Pavlenko, T.O. Busko, A.M. Gaponov, O.G. Rugal, L.I. Kurochka, P.P. Ilyin, S.V. Marysyk *Kyiv national university, Kyiv, Ukraine*
P3	**Optoelectronic and magnetic properties of RE= Sm, Eu, Gd, and Er doped zinc sulphide** H. HEDJAR, S.DERKAOUI, A.H.TABTI, A.BOUKORTT *Elaboration and Characterization Physico-Mechanical and Metallurgical of Materials Laboratory (ECP3M), Abdelhamid Ibn Badis University-Mostaganem. Route Nationale N◦11, Kharrouba, 27000, Mostaganem, Algeria; Tissemsilt University, Algeria*
P4	**Synthesis, Characterization, and Antimicrobial Evaluation of SiO2/5-ASA and SiO2/5-ASA/Ag Nanomaterials** Miljana M. Dukić, Katarina Isaković, Valentina Nikšić, Dušan N. Sredojević, Vesna M. Lazić *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*
P5	**3D statistical tolerance synthesis in mechanical assemblies** Said Boutahari, Mustapha El Mouden, Mouhssine Chahbouni *TSI laboratory, Higher school of technology, Sidi Mohammed Ben Abdellah University Imouzzer street, BP 2626 (30000), Fez, Morocco*
P6	**Development and characterization of honokiol-loaded liposomes** Karolina Olechowska *Department of Environmental Chemistry, Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387, Kraków, Poland*

P7	**Development of new type core-shell thermochromic pigments based on selected triarylmethane dyes** Bartosz Kopyciński, Alicja Duda, Sebastian Jurczyk, Grażyna Kamińska-Bach, Małgorzata Zubielewicz, Katarzyna Jaszcz *Łukasiewicz Research Network – Institute for Engineering of Polymer Materials and Dyes, M. Skłodowskiej-Curie 55 St., 87-100 Toruń, Poland; Doctoral School, Silesian University of Technology, Akademicka 2A St., 44-100 Gliwice, Poland; Łukasiewicz Research Network – Institute of Non-Ferrous Metals, gen. J. Sowińskiego 5 St., 44-100 Gliwice, Poland; Department of Physical Chemistry and Technology of Polymers, Silesian University of Technology, ks. M. Strzody 9 St.,44-100 Gliwice, Poland*
P8	**Water-based organic coatings with bioactive and camouflage properties for the protection of military equipment** Bartosz Kopyciński, Ewa Langer, Maja A. Zaczek-Moczydłowska, Andrzej Hudecki, Alicja Hryniszyn, Mariola Bodzek-Kochel, Marek Łos *Łukasiewicz Research Network – Institute for Engineering of Polymer Materials and Dyes, M. Skłodowskiej-Curie 55 St., 87-100 Toruń, Poland; Doctoral School, Silesian University of Technology, Akademicka 2A St., 44-100 Gliwice, Poland; Biotechnology Centre, Silesian University of Technology, B. Krzywoustego 8 St., 44-100 Gliwice, Poland; Łukasiewicz Research Network – Institute of Non-Ferrous Metals, gen. J. Sowińskiego 5 St., 44-100 Gliwice, Poland*
P9	**PLGA-based nanoparticles for targeted drug delivery in Immuno-Oncology therapy** Inês S. Pinto, Annalee W. Nguyen, Jennifer A. Maynard, Henrique Faneca *University of Coimbra, Institute for Interdisciplinary Research, Doctoral Programme in Experimental Biology and Biomedicine (PDBEB), Portugal; Center for Neuroscience and Cell Biology, University of Coimbra, 3004-504 Coimbra, Portugal; Department of Chemical Engineering, University of Texas, Austin, TX 78712, USA; Institute of Interdisciplinary Research (III), University of Coimbra, Casa Costa Alemão - Pólo II, 3030-789 Coimbra, Portugal*
P10	**Activated carbons from biomass for sustainable adsorption of emerging contaminants in water treatment** Tayra R. Brazil, Valentina Silva, María V. Gil, Edson C. Botelho, Vânia Calisto *Department of Materials and Technology, São Paulo State University, Guaratinguetá, Brazil; Department of Chemistry and CESAM, University of Aveiro, Aveiro, Portugal; Instituto de Ciencia y Tecnología del Carbono, INCAR-CSIC, Oviedo, Spain*
P11	**Effect of isothermal aging on the microstructural evolution in Ti-6Al-4V titanium alloy: experimental investigation and thermokinetic simulation** Nabil Kherrouba, Walid Bedjaoui, Malek Hebib, Idir Hadji *Research Center in Industrial Technologies CRTI, P. O. BOX 64, Cheraga 16014, Algiers, Algeria*

P12	**Chitosan nanoparticles included different doses of copper oxide nanoparticles produced by molasses: Investigating electrical conductance and antibacterial attributes** Noof A. Alenazi *Department of Chemistry, College of Science and Humanities in Al-Kharj, Prince Sattam bin Abdulaziz University, Al-kharj 11942, Saudi Arabia*
P13	**Investigation of local friction and surface potential properties of copper and mild steel under corrosion by atomic force microscopy** Igor Bdikin, Ricardo Beja, António Pereira *TEMA: Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal; LASI—Intelligent Systems Associate Laboratory, Guimarães, Portugal*
P14	**Antibacterial effect of ginger oil extract fixed in fluorohydroxyapatite** Maissa AGSOUS, Hafit KHIREDDINE, Sabeha YALA *Faculty of Technology, University of Bejaia, Targa Ouzemour, Algeria*
P15	**Application of magnetic TiO2 /Carbon Quantum Dots composites for the photocatalytic removal of antibiotics from water** Valentina Silva, Nuno J. O. Silva, Goreti Pereira, Marta Otero, Vânia Calisto, Diana L. D. Lima *CESAM & Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal; Department of Physics & CICECO, University of Aveiro, 3810-193 Aveiro, Portugal; Departamento de Química y Física Aplicadas, Universidad de León, 24071 León, España; H&TRC - Health & Technology Research Center, Coimbra Health School, Polytechnic University of Coimbra, 3046-854 Coimbra, Portugal*
P16	**Using CuBiO4/CuO Photocathodes to Avoid Hydrogen Evolution and Promote CO2 Reduction in a Glycerol Microfluidic Fuel Cell** Maria-Victória S. Silva, Silvio M. Mazarin, Daniel F. Costa-Filho, Adailton C. Nogueira, Heberton Wender, Cauê A. Martins *Institute of Physics, Universidade Federal de Mato Grosso do Sul, CP 549, 79070-900, Campo Grande, MS, Brazil*
P17	**Eco-Friendly Synthesis of Iron Oxide Nanoparticles and Their Application to the Removal of Arsenic and Lead from Mining-Contaminated Soils** Erico Carmona, Aliro Villacorta, Felipe Carevic, Lucas Hernández, Cynthia Rojo, Ricard Marcos *Arturo Prat University, Renewable Natural Resources Faculty, Huayquique Campus, 1100000, Iquique, Chile; Universitat Autònoma de Barcelona, Departamento de Genetica i de Microbiología, 08193 Bellaterra (Cerdanyola del Valles), Spain*

P18	**Thermal Analysis of TIG Welding: Experimental Study and Comparison with FE and FD Numerical Methods** Abdel Halim Zitouni, Mouloud Aissani, Pierre SPITERI , Younes Benkheda *Research Center in Industrial Technologies CRTI P.O.BOX 64, Cheraga 16014 Algiers, Algeria; IRIT, INP-ENSEEIHT, 2 Rue Charles Camichel 31000, Toulouse, France; Département de Génie Mécanique, Université de Blida1, BP 270, Route de Soumaa, Blida, Algérie*
P19	**AIE-Active Nanoprobes for Rapid and Selective Fluorescence Identification of Gram-Positive Bacteria** Arshad Khan, Ibraheem Bushnak, Rizwan Ali *Nanomedicine Department & core facility, King Abdullah International Medical Research Center (KAIMRC) King Saud Bin Abdulaziz University for Health Sciences, Riyadh 11426, Kingdom of Saudi Arabia*
P20	**A comparison of HPPC and PEIS test methodology for determination of LFP cells performance** Marko Viskić, Željko Ban, Zoran Mandić *Department of Electrochemistry, Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10000 Zagreb, Croatia; Department of Control and Computer Engineering, Faculty of Electrical Engineering and Computing, University of Zagreb, Unska 3, 10000 Zagreb, Croatia*
P21	**Self-trapped Polaron Signatures In Ligand-assisted Lead Halide Perovskite Nanocrystals** S. K. Jakka, T. Udaybaskarrao, R. Vidyasagar *I3N & Department of Physics, University of Aveiro, Aveiro 3810-193, Portugal; Institute of Fundamental and Frontier Sciences, UESTC, Chengdu 610054, China; CICECO & Physics Department, University of Aveiro, Aveiro 3810-193, Portugal*

Plenary lectures

High-performance electrochemical sensors to tackle microplastics and PFAS

Ajeet Kaushik

Department of Civil and Environmental Engineering, Florida Polytechnic University, Lakeland, Florida-USA

In the age of growing industrialization and capitalism, the use of high-performance materials is well adopted but several important aspects during the preparation and after application needed to be evaluated to make sure their effects of ecosystem. On this track, the advanced application of plastic and per- and polyfluoroalkyl substances (PFAS) materials cannot be overlooked but their related consequences are also alarming. Because plastic changes to microplastic (long-lasting pollutant) under several conditions and PFAS also etched out and integrated with environment as a forever chemical. To keep tracking and monitoring, the efficient sensing of MPs and PFAS is essential, and it should be in the setting of point-of-care (POC) to support sustainability.

To meet some of the above discussed requirements, my laboratory is exploring high-performance electrochemical sensing of MPs and PFAS. To achieve the desired sensing parameters, we are focused on exploring several interfacing and detection approaches. Presently smart materials-based sensing technology interfaced with other tools like the Internet of Things (IoT, 5th generation sensing) and artificial intelligence (AI, 6th generation sensing) are our focus to develop point-of-care (POC) electrochemical sensors. Our approach consists of customized electrodes interfaced with the smart electrochemical analyzer that can be operated using a smartphone. Recently, we have developed a Molecularly Imprinted Polymers (MIPs)-based electrochemical sensing of MPs (polystyrene and polyethylene) and PFAS in water samples at a low concentration (ppb level). Such developed smartphone-EA@MIP-based electrochemical sensing systems can detect MPs and PFAS on-site field to analyze the situation and decision-making timely.

Optimizing response of printable magnetorheological elastomers for advanced applications

Senentxu Lanceros-Méndez [1, 2, 3]

[1] BCMaterials, Basque Center for Materials, Applications and Nanostructures, UPV/EHU Science Park, 48940 Leioa, Spain
[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

In the increasingly interesting area of stimuli-responsive materials, magnetorheological materials are of particular interest, as they allow to modify their mechanical properties (e.g. elastic moduli) as a response to a magnetic field. Magnetorheological elastomers (MREs), in particular, are composed of a polymeric matrix that provides the base mechanical properties and a magnetic filler responsible of the magnetoactive response.

Further, additive manufacturing (AM) technologies enables printing of complex structures through different techniques, such as direct ink writing (DIW), which allows manufacturing with higher resolutions and widens the scope of application of MREs to other areas such as micro and nanoelectronics, healthcare, automotive or micro-robotics. Nevertheless, traditionally used microparticles are a limiting factor, since the resolution is limited by their size. Thus, being able to fabricate MREs with nanoparticles (NPs) is of critical importance.

The magneto-mechanical properties of SEBS-based MREs are presented by exploring the different possibilities in terms of NP selection. The effect of the magnetic properties, concentration, shape, and orientation of the NPs in the magnetorheological response have been explored to gain a clear understanding of how the specific design of the materials allows to tune the active functional properties. We have also shown the possibility of fabricating self-sensing systems by combining magnetic NPs and multi-walled carbon nanotubes in a single ternary composite, which combines magnetorheological and piezoresistive properties.

Overall, it will be shown how properly tailor MRE response allows a wide range of applications in areas including soft-robotics, biomedicine and aerospace.

Acknowledgements

Fundação para a Ciência e Tecnologia (FCT): UID/04650/CFUM-UP, POCI-01-0247-FEDER-046985, 2022.03931. PTDC. Advanced Materials program supported by MCIN, European Union NextGenerationEU (PRTR-C17.I1), Basque Government: IKUR and Elkartek programs. PID2022-138572OB-C42 funded by MCIN/AEI/10.13039/501100011033/FEDER, UE and BIOIMP_ACE_MAS_6_E, European Union, Interreg VI-A Spain-Portugal Program (POCTEP) 2021-2027.

Magnetic metallic nanoparticles produced from oxide precursors via pyrolysis without the use of added reducing agents or a reductive atmosphere

Robert C. Pullar [1] * and César de Julián Fernández [2]

[1] Dipartimento di Scienze Molecolari e Nanosistemi (DSMN), Università Ca' Foscari Venezia, Venezia Mestre, Venezia (VE) 30172, Italy
[2] Istituto dei Materiali per l'Elettronica e il Magnetismo - CNR-IMEM, Parco Area delle Scienze 37/A, Parma 43124, Italy
* Corresponding/Presenting author: robertcarlyle.pullar@unive.it

It is well known that magnetic metallic nanoparticles (NPs) based on iron can be produced from the reduction of iron oxides. In this process, Fe^{3+} is reduced to Fe^{2+} and finally metallic Fe^{0} with treatment in a reducing atmosphere such as hydrogen or carbon monoxide gas, typically at temperatures of 550-1000 °C. However, here we report the conversion of α-Fe_2O_3 into metallic α-iron NPs after heating to 1000 °C / 2h under only an N_2 atmosphere in a pyrolysis furnace, with no reducing atmosphere or added reducing agents required. Futhermore, metallic CoFe NPs were also produced from iron and cobalt nitrate/oxide precursors under similar conditions. These metallic NPs were extremely soft magnets, with coercivity (H_c) of 60-80 Oe (4.77-6.37 kA m^{-1}), but they were not superparamagnetic, with a remnant magnetisation (M_r) ~3-5% of the saturation magnetisation (M_s). Both had very high magnetisations at 1.7 T of 195 emu g^{-1} (A m^2 kg^{-1}) for the α-Fe NPs and 215 emu g^{-1} (A m^2 kg^{-1}) for the CoFe NPs. These were produced under the HYPERMAG project (*HYbrid ferrite nanocomposites for novel rare earth free PERmanent MAGnets*), and could be ideal materials for magnetic coupling with hard magnetic ferrite NPs to create hybrid permanent magnets with increased magnetisation. This work was developed in the framework of the PRIN-PNRR project HYPERMAG (prot. P2022RRRT4, CUP H53D23007990001) funded by the European Union – NextGenerationEU.

What is up with Nature? One Mechanical Engineer’s View

Philip LeDuc
Departments of Mechanical Engineering, Biomedical Engineering, Computational Biology, and Biological Sciences, Carnegie Mellon University, USA

I have always been interested in examining whether seemingly unconnected areas of my life actually have intersections. For example, two areas that have always interested me are the mechanics of machines such as taking apart lawn mowers in my youth and the wonders of nature. While they seem unconnected, I wonder what are their commonalities, which has led me to work on this intersection for over 2 decades. Here I will present how my lab has been looking for nature that are threaded throughout life. My lab approaches this by envisioning different biological organisms as “systems” and is examining how these unconnected systems intersect. We use our approaches as engineers for investigating these systems in nature looking for unifying principles with some of the same fundamental approaches used on machines such as planes, trains, and automobiles. I work with a diversity of biological systems ranging from mammalian cells to microorganisms to plants to animals and we apply principles from mechanical engineering fields (e.g. solid mechanics, control theory, fluidics, heat transfer, design) to understand how these principles may apply across diverse nature-based systems. My goal with my projects is to tackle grand challenges so my work includes areas like improving health, sustainable energy, clean water, understanding evolution, and even art. We pursue these goals through developing and utilizing unique custom-built systems including biotechnology, robotics, artificial intelligence, and computational biology. These intersections are especially fascinating to me as biological systems have evolved for distinct reasons (the “initial and boundary conditions” are different). In addition, as an engineer, I truly am interested in building new systems from the knowledge that we obtain thus, I will also present how our lab thinks about these nature-inspired design principles toward translational efforts.

Biomimetic hydrogels and engineering strategies for functional tissue regeneration

Ana Marina Ferreira-Duarte *

School of Engineering, Newcastle University, Newcastle-Upon-Tyne, UK
*e-mail: ana.ferreira-duarte@newcastle.ac.uk

The extracellular matrix (ECM) plays a central role in regulating cellular behaviour, immune modulation, and tissue homeostasis. Its degradation or dysfunction underpins many degenerative conditions, making ECM-mimetic biomaterials a cornerstone of regenerative medicine. Natural polymers such as collagen, alginate, fibrin, and hyaluronic acid offer structural and biochemical similarity to the ECM, along with tuneable properties that make them ideal for engineering dynamic, functional tissue microenvironments.

In this talk, I will present our integrated approach to developing bioinspired hydrogels and natural-material-based scaffolds that emulate ECM function across diverse tissue types. Our early work on collagen systems for bone repair [1] established critical design principles that informed subsequent developments in bio-instructive hydrogels for soft tissue, bone and cartilage regeneration [2-5]. We will discuss strategies to tune material composition, degradation, and immune interaction [4], as well as the importance of cell density and microarchitecture in achieving functionality and tissue maturation [5-11]. Furthermore, the synergy between natural-based materials and porous scaffolds, as well as surface coatings to mimic bone microenvironments, will be explored [6, 8, 11, 12].

Collectively, our work demonstrates how nature-based biofunctional materials, when coupled with advanced biofabrication technologies, can guide cellular organisation, tissue morphogenesis, and regenerative outcomes. These innovative materials and platforms move us closer to advanced and adaptive therapeutic strategies in regenerative medicine.

References

1. *Acta Biomaterialia*, 2012, **8**(9), 3191–3200.
2. *Materials Science and Engineering: C*, 2018, **91**, 236–246.
3. *Journal of Functional Biomaterials*, 2023, **14**(10), 495.
4. *Acta Biomaterialia*, 2023, **155**, 1–18.
5. *Scientific Reports*, 2019, **9**(1), 14630.
6. *Biofabrication*, 2019, **11**(1), 015014.
7. *BioDesign and Manufacturing*, 2022, **5**(3), 512–528.
8. *Biomaterials Advances*, 2023, **153**, 213532.
9. *Biomaterials Science*, 2021, **9**(12), 4246–4259.
10. *Frontiers in Bioengineering and Biotechnology*, 2024, **12**, 1391728.
11. *International Journal of Molecular Sciences*, 2024, **25**(20), 11131.
12. *ACS Biomaterials Science and Engineering*, 2025, **11**(5), 2690–2704.

Estimation of the degree of antisite disordering of magnetoactive ions in $Sr_2FeMoO_{6-\delta}$ by means of the intensity of the X-ray peak (101)

Gunnar Suchaneck*, Evgenii Artiukh

TU Dresden, Institute for Solid-State Electronics, 01062 Dresden, Germany

* *Phone/fax: +49 351 463 35281/-, e-mail address: gunnar.suchaneck@tu-dresden.de*

Strontium ferromolybdate ($Sr_2FeMoO_{6-\delta}$, SFMO) double perovskite is a promising candidate for room-temperature spintronic applications due its high Curie temperature (around 415 K) and near 100% spin polarization at low temperatures. Nevertheless, SFMO has not yet found wide application in spintronics. This is attributed to the low reproducibility of its magnetic properties, which partially originates from their strong dependence on the ordering degree of Fe and Mo ions in the B' and B" sublattices of double perovskite $A_2B'B"O_6$.

In this work, we have considered an express method of determining the degree of disorder in strontium ferromolybdate. The sublattice occupation with Fe and Mo ions has been estimated for stoichiometric and nonstoichiometric SFMO with a 5% Fe and Mo excess, respectively. We have calculated the intensity ratio between the superstructure (101) and the most intense (112 + 200) peaks. The calculated curves have been fitted to an analytical expression of a similar case known from literature. The calculation results obtained using the proposed method are within a ± 25 % agreement with Rietveld analysis of experimental data. Thus, this method can be used as an alternative to Rietveld analysis if the exposure time during X-ray diffraction experiment was insufficient. We have discussed the dependence of the I(101)/I(112 + 200) peak intensity ratio on various factors including instrumental broadening of diffraction peaks, peak twinning due to grain size reduction, thin film lattice parameter variation due to substrate lattice mismatch (in case of thin films) and lattice parameter variation due to oxygen vacancies.

The described in this work method allows to reduce X-ray exposure time while ensuring high reliability when applied to near-stoichiometric SFMO specimens characterized by an approximately equal iron-to-molybdenum ratio. The relevance of the method is the evaluation of the degree of superstructure ordering in $Sr_2FeMoO_{6-\delta}$ without large time consumption for X-ray diffraction pattern recording and Rietveld data processing, which may be essential when dealing with large amounts of experimental samples.

Material-related problems of neuromorphic technologies

Nikolai A. Sobolev
Departamento de Física & i3N, Universidade de Aveiro, 3810-193 Aveiro, Portugal,
e-mail: sobolev@ua.pt

Advancements in materials science have been instrumental in the progression of neuromorphic technologies. However, existing neuromorphic hardware often relies on rigid and energy-intensive fabrication processes.

The inevitability of a revolution in electronic technologies is dictated by the emergence of new paradigms of electronics which cannot be implemented on existing hardware. Traditional computing architectures struggle with energy efficiency, scalability, and adaptability, particularly as AI and data-intensive applications demand greater computational power. Machine learning tends, in the limit, to consume all the power produced in the world, and this development model is costly, inefficient and unsustainable. Neuromorphic computing presents a promising alternative by enabling real-time, low-power processing. Crucial for this development are materials being able to implement bio-inspired functions. There is an urgent need for innovative materials and device architectures that can bridge this gap while ensuring scalability and eco-friendliness.

Thus, the presentation is dedicated to the material problems of neuromorphic technologies and aims to review a wide range of theoretical and experimental results in this field.

Invited speakers

I1. Recent Advancements in Photocatalysis Using Nanocomposites

Vikram Uttam Pandit*

Haribhai V. Desai College of Arts, Science and Commerce (Autonomous) Pune, India

**Email: vikramupandit@gmail.com*

Abstract: Recent advancements in photocatalysis have increasingly focused on the development and application of nanocomposites to enhance photocatalytic efficiency under visible light. Nanocomposites, formed by integrating semiconductor materials with other nanostructured components such as metals, metal oxides, carbon-based materials (e.g., graphene, carbon nanotubes), and metal–organic frameworks (MOFs), offer superior charge separation, extended light absorption, and improved surface reactivity. These hybrid structures exploit synergistic effects among their constituents, enabling better utilization of the solar spectrum and reduced electron-hole recombination. Innovative synthesis techniques such as hydrothermal methods, sol-gel processes, and atomic layer deposition have enabled precise control over nanocomposite morphology and composition. Recent research has highlighted significant progress in heterojunction-based nanocomposites like Z-scheme and S-scheme systems, which preserve redox potential while achieving enhanced photocatalytic activity for applications such as water splitting, CO_2 reduction, and pollutant degradation. Moreover, doping with rare earth elements and plasmonic nanoparticles has further contributed to increased visible-light response and catalytic durability. These advances pave the way for sustainable and energy-efficient solutions in environmental remediation and renewable energy production. Future research is anticipated to focus on scaling up production, enhancing long-term stability, and exploring novel material combinations through machine learning and high-throughput screening.

I2. Engineering ceramic thermoelectrics: from design to functional performance

Andrei V. Kovalevsky[1, *], Diogo Lopes[1,2], Parisa Amirkhizi[1], Miguel A. Vieira[1], Nuno Ferreira[2], Aleksey A. Yaremchenko[1], Shahed Rasekh[1], Wenjie Xie[3,4], Anke Weidenkaff[3,4], Andres Sotelo[5]

[1]*CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal*
[2]*i3N, Physics Department, University of Aveiro, 3810-193 Aveiro, Portugal*
[3]*Materials and Resources, Department of Materials and Earth Sciences, Technical University of Darmstadt, Darmstadt 64287, Germany*
[4]*Fraunhofer Research Institution for Materials Recycling and Resource Strategies IWKS, Alzenau 63755, Germany*
[5]*INMA (CSIC-Universidad de Zaragoza). Mª de Luna, 3. 50018 Zaragoza, Spain*
[*] akavaleuski@ua.pt

Thermoelectric (TE) technology enables the direct conversion of heat flux into electricity and offers a solid-state alternative for both energy harvesting and cooling applications. It is particularly attractive for recovering waste heat in industrial processes, transportation, and remote systems, due to its reliability, scalability, and maintenance-free operation. Ceramic TE materials, especially oxide-based systems, stand out for their excellent thermal and chemical stability, combined with the abundance of constituent elements, key features for high-temperature operation and long-term sustainability. In contrast to conventional TE materials, which often rely on scarce, toxic elements and thermally unstable compositions, ceramics offer a path towards environmentally friendly and cost-effective solutions. However, unlocking their full potential requires advanced design strategies and tailored processing approaches to overcome challenges related to electrical and thermal performance, as well as microstructural control. This work reviews the current state-of-the-art and recent trends in the development of ceramic-based thermoelectric materials. It discusses a range of strategies for material design and processing, including composite architectures, defect engineering, cationic substitution, redox tailoring, and advanced techniques such as laser processing, among others.

Acknowledgements

This work was developed within the scope of the project CICECO-Aveiro Institute of Materials, UIDB/50011/2020 (DOI 10.54499/UIDB/50011/2020), UIDP/50011/2020 (DOI 10.54499/UIDP/50011/2020) & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC), and the project MeXTSus, Nº 16602, supported by FEDER and national funds, under the Call for Applications No. MPr-2023-12. Diogo Lopes acknowledges the PhD scholarship by FCT (grant 2020.06454.BD). Miguel Vieira acknowledges the PhD scholarship by FCT (grant 2022.12347.BD).

I3. Comparison of functionality and sensitivity of surface-enhanced Raman scattering and surface plasmon resonance sensors for DNA identification: Identification of BRCA1 gene mutation variants in clinical samples

Andrzej Kudelski *

Faculty of Chemistry, University of Warsaw, 02-093 Warszawa, Poland

**phone: +48-225526401, fax: +48-225526428, e-mail address: akudel@chem.uw.edu.pl*

The deoxyribonucleic acid (DNA) is the carrier of genetic information for all living organisms. Even a small mutation in DNA sentence can cause many diseases. Therefore, developing sensitive, fast and precise methods for detection of DNA mutations is very important from a practical point of view. Promising methods for detection of specific DNA fragments are surface-enhanced Raman scattering (SERS) spectroscopy [1-4] and surface plasmon resonance (SPR). In this contribution we describe construction and tests with clinical samples of SERS and SPR sensors for the identification of six the most popular in Poland variants of BRCA1 gene mutations. Both sensors were based on the selective hybridization of target DNA with the capture DNA immobilized on plasmonic substrates (see Figure 1). Moreover, in both sensors the same thiolated capture DNA was used.

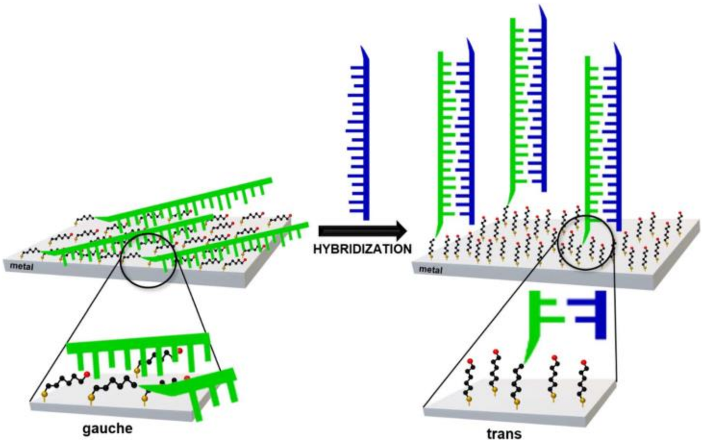


Figure 1. Scheme of the SERS DNA sensor based on rearrangement of the alkanethiol chains (alkanethiolate linking moiety of single stranded DNA and 6–mercaptohexan–1–ol). Reprinted from ref. [3]. CC BY license.

The mutation identification process using SPR detector relied on the shape of the SPR sensorgrams, whereas for the SERS sensors, the intensity of the Raman band at about 715-735 cm^{-1} (this band is due to the superimposition of mainly the band due to the ν(C−S) vibration of the alkanethiol chain in the *trans* conformation and the band due to the breathing vibration of adenine) was used as an analytical signal. The demonstrated biosensors are characterized by the low detection limit at the level of $pg \cdot \mu L^{-1}$, wide analytical range and high selectivity. It was found that for different DNA sequences, a SPR or SERS sensor achieves greater detection sensitivity, which means that the selection of the optimal sensor type depends on the sequence of the target DNA. The proposed analytical approaches demonstrated completely new capabilities of SPR and SERS techniques and new insights into gene mutation detection

Acknowledgments

This work was financed by the National Science Centre, Poland, project No. 2019/35/B/ST4/02752.

References

[1] Y. He, S. Su, T. Xu, Y. Zhong, J. A. Zapien, J. Li, C. Fan, and S.-T. Lee, *Nano Today,* **6**, 122 (2011).
[2] S. He, K.-K. Liu, S. Su, J. Yan, X. Mao, D. Wang, Y. He, L.-J. Li, S. Song, and C. Fan, *Analytical Chemistry*, **84**, 4622 (2012).
[3] A. Michałowska, A. Gajda, A. Kowalczyk, J. L. Weyher, A. M. Nowicka, and A. Kudelski, *RSC Advances*, **12**, 35192 (2022).
[4] A. Kowalczyk, J. Krajczewski, A. Kowalik, J. L. Weyher, I. Dzięcielewski, M. Chłopek, S. Góźdź, A. M. Nowicka, and A. Kudelski, *Biosensors and Bioelectronics*, **132**, 326 (2019).
[5] A. Gajda-Walczak, A. Potęga, A. Kowalczyk, S. Sęk, A. Kowalik, S. Zięba, A. Kudelski, and A. M. Nowicka, *Scientific Reports*, **13**, 7316 (2023).
[6] L. G. Carrascosa, A. Calle, and L. M. Lechuga, *Analytical and Bioanalytical Chemistry*, **393**, 1173 (2009).

I4. Contact Angle Measurement with Simplified Approach and Applications

Serbülent TÜRK *, Burak ÜNLÜ
Sakarya University, Biomedical, Magnetic and Semiconductor Materials Research Center (BIMAS-RC), 54187, Sakarya, Turkey

* *+90 264 295 31 83, serbulentturk @sakarya.edu.tr*

Contact angle measurement, which has an important place in determining the surface structure, is a valuable characterization for analyzing surface properties.

In addition to the use of complicated devices in measuring the contact angle, low-cost methods where users can prepare the conditions of the environment (humidity, temperature, etc.) without the need for high-cost devices are not very well known, but are available in the literature [1,2].

In this study, Ti surface was coated with bio-ceramics and the contact angles of different coating materials were measured with a user-friendly setup using the needle-drop method. The drop-surface properties of the coatings were successfully determined thanks to a cost-effective contact angle measurement setup that will benefit researchers in disciplines such as materials science, chemical engineering, and physical chemistry.

References

1. Khan, M.S.; Wani, A.A.; Jan, Q.; Bhat, M.M.; Kuchey, M.Y.; Sheikh, U.R.; Sofi, F.A.; Bhat, M.A. Smartphone-Assisted Contact Angle Measurements: A Simple Approach to Determine the Critical Micelle Concentration of Surfactants. *J. Chem. Educ.* **2024**, *101*, 1198–1203, doi:10.1021/acs.jchemed.3c00953.
2. Zou, Y.; Ross, N.; Nawaj, W.; Borguet, E. A Simplified Approach for Dynamic Contact Angle Measurements. *J. Chem. Educ.* **2024**, *101*, 3883–3890, doi:10.1021/acs.jchemed.4c00146.

I5. Supramolecular one- and two-dimensional peptide nanostructures for energy storage and harvesting

P. Zelenovskii[1,*], R. Ferreira[1], F. Hagiwara[1],
P. Brandão[2], A. Kholkin[1], S. Kopyl[1], F. Figueiredo[1]
[1]Department of Physics and CICECO, University of Aveiro, 3810-193 Aveiro, Portugal
[2]Department of Chemistry and CICECO, University of Aveiro, 3810-193 Aveiro, Portugal
[*]E-mail address: zelenovskii@ua.pt

Supramolecular peptide-based materials are promising functional elements for a wide range of bioelectronic devices, such as biosensors, energy harvesters, and energy storage devices [1,2]. These materials are inherently eco-friendly, offer a remarkable chemical diversity and self-assemble into hierarchical supramolecular nanostructures with unique physical properties. Though two-dimensional (2D) peptide crystals and thin films have the greatest practical importance [3,4], they still remain the least studied peptide structures.

In this work, we created nanotubes and 2D layered crystals based on diphenylalanine (FF), dileucine (LL), and phenylalanine-glutamic acid (FE), studied their structure and morphology, and evaluated their cathodic and anodic properties. Estimations show an outstanding Li capacity of FF nanotubes about 375 mAh/g comparable with the capacity of graphite (372 mAh/g). Moreover, large-area (c.a. 500 mm^2) crystalline thin films of LL (thickness below 400 nm) created by the spin-coating technique, demonstrate high piezoelectric coefficient d_{33} c.a. 18 pm/V comparable to that of other organic materials. These results demonstrate the potential of peptide-based nanomaterials for various energy applications.

This work was developed within the projects CICECO-Aveiro Institute of Materials (UIDB/50011/2020, UIDP/50011/2020, LA/P/0006/2020) and “BioPiezoSensor” (2022.03781.PTDC, DOI 10.54499/2022.03781.PTDC) financed by national funds through the FCT and FCT/MEC (PIDDAC). The authors are grateful for the financial support granted by the Recovery and Resilience Plan (PRR) and by the Next Generation European Funds to Universidade de Aveiro, through the Agenda for Business Innovation “NGS - Next Generation Storage” (Project nº2 with the application C05-i01.01/2022) and by the Horizon Europe Framework Program (HORIZON-TMA-MSCA-SE, Project PIEZO 2D, No. 101131229).

References

[1] J. Zhao, Q. Liu, X. Tong, et al., *Adv. Funct. Mater.*, **34**, 2401466 (2024).
[2] P. Zelenovskii, K. Romanyuk, et al., *Adv. Funct. Mater.*, **31**, 2102524 (2021).
[3] K. Romanyuk, V. Slabov, et al., *Appl. Mater. Today*, **26**, 101261 (2022).
[4] D. Alikin, V. Yuzhakov, et al., *ACS Biomater. Sci. Eng.*, **9**, 6715 (2023).

I6. Routes for Eco-Friendly Recovery of Palladium and Platinum

Natalia Tsyntsaru[1,2,*], Henrikas Cesiulis[2]

[1] *Faculty of Chemistry and Geosciences, Vilnius University, 03225 Vilnius, Lithuania,*
[2] *Institute of Applied Physics, Moldova State University, 2028 Chisinau, Moldova.*
[*] *ashra_nt@yahoo.com*

Palladium and platinum are renowned for their exceptional physicochemical properties and play a crucial role in various industrial applications. Notably, in vehicle emission control systems, they help in the catalytic conversion of harmful gases like carbon monoxide and nitrogen oxides into less harmful emissions. As we pivot towards a circular economy, it becomes increasingly vital to investigate secondary sources of palladium and platinum, particularly from urban mines, which consist of electronic waste, catalytic converters, and other discarded products containing these precious metals. Currently, the prevalent technologies employed for the recovery of palladium and platinum are often characterized by high energy consumption, which can lead to significant operational costs. Moreover, these methods frequently result in adverse environmental impacts, including greenhouse gas and nitrogen oxides emissions, and the generation of hazardous waste. Therefore, there is an urgent need for more sustainable and efficient recovery techniques that minimize both energy use and environmental aftermath while enhancing the overall yield of metals extraction from secondary sources.

One green method is electrochemical metal recycling. Different approaches are used to achieve eco-friendly leaching, e.g., recovering palladium from spent catalysts through a combination of mild acidic leaching and photodeposition on ZnO nanoparticles or carbon-based electrodes. This study aims to elucidate the corrosion behaviour of Pd and Pt by measuring key electrochemical corrosion parameters, including corrosion potential, corrosion current density, and polarization resistance, in 1 M aqueous solutions of various ligands known to facilitate the formation of complex compounds. Using linear sweep voltammetry and electrochemical impedance spectroscopy, experiments were conducted at controlled temperatures of 20 °C and 60 °C.

Acknowledgment. This research has received funding from the Lithuanian Research Council Project S-MIP-24-11.

I7. A-site substituted Aurivillius Rare earth Perovskite structures: A pathway to tunable optoelectronic properties

K. Pavani

i3N & Department of Physics, University of Aveiro, Aveiro 3810-193, Portugal

**Corresponding author email: pavani_physics@yahoo.co.in; pavani@ua.pt*

Aurivillius compounds comes under subclass of layered perovskite structures and are known for their unique alternative stacking of $(Bi_2O_2)^{2+}$ and $(WO_4)^{2-}$ octahedrons layers. With a specific A-site substitution with alkali earth or rare earth (RE^{3+} = Gd^{3+}, La^{3+}, Eu^{3+}, Er^{3+}, Tm^{3+}, Yb^{3+} etc.,) ions lead to band gap tunability and improved optical response. Such modifications also influence interlayer and intra layer ion interactions with lower octahedron perturbations. In addition, RE^{3+} 4f electron configuration, rich energy level distribution and $5s^2$, $5p^6$ shielding effect would provide promising choice for A-site substitution. In the present study, a series of RE^{3+} substituted (A-site) Bi_2WO_6 structures were employed and their photo responsive characteristics were analysed in detailed. The optimized materials were demonstrated for a variety of applications such as latent fingerprint and flexible screen-printing polymers. To assess the structural and morphological properties of these materials, we performed various techniques, including X-ray diffraction (XRD), X-Ray photo-electron spectroscopy (XPS), Raman spectroscopy, Fourier Transform Infra-red (FT-IR ATR), Diffuse Reflectance Spectroscopy (DRS) and Field Emission Scanning / Transmission Electron Microscopy (FE-SEM/TEM). The present compound is iso-structural to the high-temperature phase (HT) of Bi_2WO_6. Spectroscopic properties such as upconversion (UC) and downshifting (DS) processes were discussed with theoretical interpretations. This study provides a promising foundation for designing the rare-earth perovskites and suitable implementation to sensor technology.

I8. High sensitive setup of gold nanorods substrates for explosives detection using surface enhanced Raman spectroscopy

Sultan Ben Jaber*

Forensic Chemistry, Department of Forensic Science, King Fahad Security College, Riyadh 13232, Saudi Arabia
**Tel: (00966)557725566, Email: jabers@kfsc.edu.sa.*

Abstract

Surface enhanced Raman spectroscopy (SERS) is a sensitive analytical technique that has been widely utilised for detection of trace levels of organic species. The detection of trace levels of poor vapour pressure molecules such as explosives is a critical challenging due to the low concentration of adsorbed molecules on the surface sites of the SERS substrate. In this work, gold nanorods were fabricated with analyte samples and provided highly sensitivity of SERS detection along with low limit-of-detection (LOD) for explosives down to pM of 2,4- dinitrotoluene (DNT) and nM of both 2,4,6-trinitrotoluene (TNT) and 1,3,5-trinitroperhydro-1,3,5-triazine (RDX) with highly specificity. The sensitivity of the detection was developed by optimising the adsorption of the molecules on nanorods sites , where nanorods and analyte solution were mixed followed by rigorous stirring. This procedure allowed extra molecules to be adsorbed on the nanorods surface, thus, high SERS enhanced has been observed with high specific identification of target probes. This approach showed a powerful method for rapid detection of explosives based SERS technique especially for illicit samples, where the enhancement factor calculated for analytes was in the range 3.17×10^{8} to 2.69×10^{11}.

Introduction

Since the discovery of Surface enhanced Raman scattering (SERS) phenomena in 1974, it has become a powerful and highly sensitive technique specially for trace- samples identification [1,2]. SERS was used effectively for detection of a wide range of analytes including biological, illicit and environmental samples [3–6]. The enhancement of Raman signals occurs by amplification of scattering photons for molecules placed on or close approximate on substrate, and most reported nanostructures that provide the highest SERS enhancement those materials containing noble metal nanoparticles that display plasmonic bands, such as gold and silver nanostructures[7,8]. In this work, gold nanorods were used as SERS substrates for trace levels of explosives samples with very limit of detection (LOD) and high selectivity for all examined explosives (DNT, TNT and RDX). The fabricated AuNRs substrate activity was first evaluated using a model analyte, Rhodamine-6G (R6G), with excellent enhancement factors (1.32×10^{11}) with limit of detection below 10^{-12}M. Similar trend has observed for selected explosives DNT, TNT and RDX, as they exhibited limit of detection of 10^{-12}M, 10^{-9}M and 10^{-9}M respectively, these results accomplished with highly specificity for all analytes. EF was calculated for all explosives and shown high values which revealed the strong enhancement for Raman signals and present an applicable approach for explosives identification at trace levels, as EFs for explosives reported in this study were 2.69×10^{11} for the 10^{-12}M sample of DNT, and 5.19×10^{8} and 8.25×10^{8} for 10^{-9}M of TNT and RDX samples respectively.

Method

AuNRs were prepared following using CTAB and $HAuCl_4$ solutions, where gold seeds have been prepared followed by growth to nano rods using $AgNO_3$ and ascorbic acid, SERS substrates where prepared via mixing analytes with the fresh nano rods, then SERS measurements were done using laser 633 nm.

Results

SERS measurements were conducted for three analytes of explosives, 2.4.6- di nitro toluene (DNT) (figure 1) , 2, 4, 6- trinitrotoluene (TNT), and Cyclotrimethylenetrinitramine (RDX). SERS data for DNT samples exhibited high sensitivity even at low concentration 10^{-12}M, as the main mode at ~1350-1390 cm^{-1} can be observed, showing the advantage of our SERS set- up in this work. TNT had shown the highest enhancement compared to other samples, which mainly attributed to the high number of molecules adsorbed on the Au substrates which increase the chance of maximizing the hotspot leading to obtain strong enhancement. SERS spectrum RDX samples shown remarkable enhancement especially for signature peaks. The most intense peak was observed at approximately 882 cm^{-1} that attributed to the asymmetric stretch breathing mode of the RDX ring.

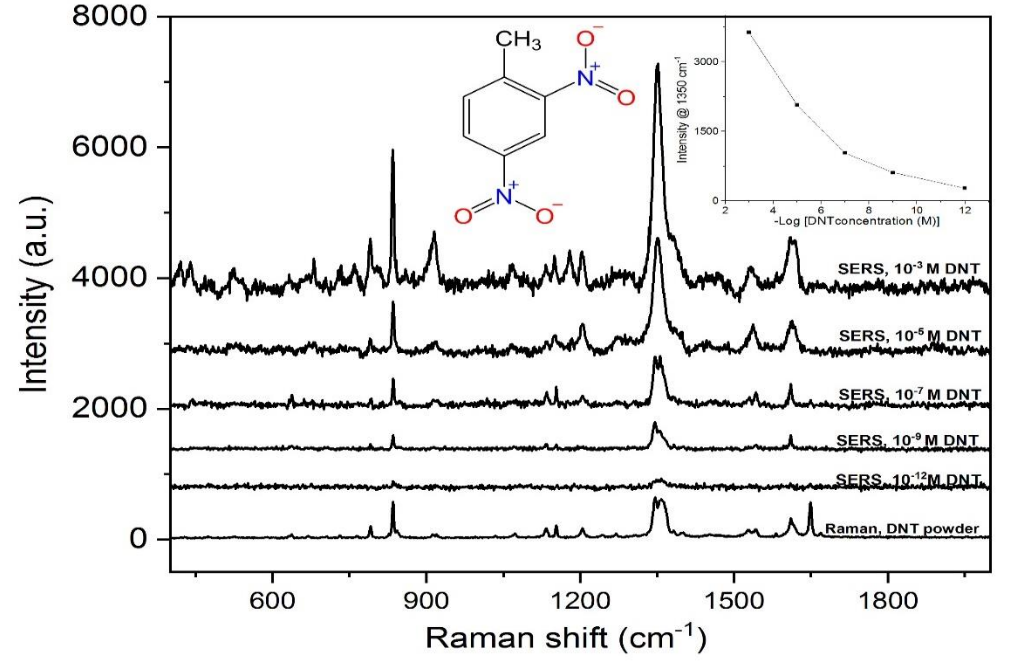


Figure 1| Raman and SERS spectra of 2, 4-di nitro toluene (DNT) on gold nanorods substrates from different concentrations in ethanol in the range 10^{-3}M to 10^{-12}M. The inset shows the relation between SERS intensity of the band 1350 cm^{-1} of DNT and samples concentration.

Discussion

there are a number of factors that affect the sensitivity and reproducibility of SERS. The most important one discussed in this work are the properties of the nanoparticles substrates. The shape and size of the nanoparticles as distributed in the substrate affect the sensitivity of the SERS. In the tests conducted, the Au nanorods of were randomly distributed and later deposited on the glass slides for air drying and SERS measurements. As a result, the detection sensitivity of the samples was reduced with the limit being 10^{-12}M for the R6G and 10^{-12} M for DNT and TNT, and 10^{-9}M for RDX. Since R6G molecules are large and have, they resulted in a high scattering with a lower cross section area of the molecules, thus, even at picomolar of R6G, SERS enhancement was remarkable compared to DNT and TNT samples.

The sensitivity of the SERS could be improved through close packing of the nanorods. The enhancement of the nanostructures (AuNRs in this work) is mainly affected by electromagnetic enhancement mechanism (EM) and chemical enhancement (CT). The two processes involve generating electrons across the analyte, as more deposited molecules, higher enhancement can be obtained. For lower concentrations, the enhancement factors were recorded high, and it is a common phenomenon to have EFs that are higher with low concentrated solutions. This can be attributed to the nature of the EF formula. The recorded values for the concentrations show varying values of the EF across different concentrations,

References

1. Halvorson, R. A. & Vikesland, P. J. Surface-enhanced Raman spectroscopy (SERS) for environmental analyses. (2010).
2. Le Ru, E. C. *Principles of surface-enhanced raman spectroscopy : and related plasmonic effects*. (Elsevier Science, 2009).
3. Aoki, P. H. B., Furini, L. N., Alessio, P., Aliaga, A. E. & Constantino, C. J. L. Surface-enhanced Raman scattering (SERS) applied to cancer diagnosis and detection of pesticides, explosives, and drugs. *Rev. Anal. Chem.* **32**, 55–76 (2013).
4. Emamian, S., Eshkeiti, A., Narakathu, B. B., Avuthu, S. G. R. & Atashbar, M. Z. Gravure printed flexible surface enhanced Raman spectroscopy (SERS) substrate for detection of 2,4-dinitrotoluene (DNT) vapor. *Sensors Actuators B Chem.* **217**, 129–135 (2014).
5. Liu, M. & Chen, W. Graphene nanosheets-supported Ag nanoparticles for ultrasensitive detection of TNT by surface-enhanced Raman spectroscopy. *Biosens. Bioelectron.* **46**, 68–73 (2013).
6. Sajanlal, P. R. & Pradeep, T. Functional hybrid nickel nanostructures as recyclable SERS substrates: detection of explosives and biowarfare agents. *Nanoscale* **4**, 3427–3437 (2012).
7. George C. Schatz and Richard P. Van Duyne, M. A. Y. Electromagnetic Mechanism of SERS. *Phys. Appl.* **103**, 19–46.
8. Le Ru, E. C. & Etchegoin, P. G. Quantifying SERS enhancements. *MRS Bull.* **38**, 631–640 (2013).

I9. Carbon Dots Driving Innovation in Health and Environmental Technologies

A. Catarina Moreira[1,2], Duarte Almeida[1,2], **Gil Gonçalves**[1,2]
[1]*Centre for Mechanical Technology and Automation (TEMA), Mechanical Engineering Department, University of Aveiro, 3810-193 Aveiro, Portugal*
[2]*Intelligent Systems Associate Laboratory (LASI), 4800-058 Guimarães, Portugal*

Carbon dots (CDs) are an emerging class of carbon-based nanomaterials characterized by their spherical shape, ultra-small size typically less than 10 nm, and chemical composition primarily consisting of carbon, nitrogen, and oxygen atoms.[1] These unique structural features endow CDs with a range of exceptional properties, including excellent biocompatibility, low toxicity, and remarkable photoluminescence. As a result, CDs have gained significant attention as versatile tools in several domains, particularly in healthcare and environmental applications.

In the field of cancer therapy and diagnostics, CDs have shown great promise. Their superior biocompatibility and tunable fluorescent properties make them ideal candidates for imaging biological structures in both in vitro and in vivo settings[2]. Additionally, CDs can be engineered for targeted drug delivery to cancer cells. Their surfaces can be functionalized with various therapeutic agents, enabling selective delivery and enhancing the efficacy of treatments such as chemotherapy and photodynamic therapy [3]. Beyond biomedical use, CDs also offer significant potential in environmental applications, including water purification and pollutant detection. CDs can adsorb heavy metals, dyes, and other harmful contaminants, making them valuable in advanced water treatment systems. Moreover, their fluorescence is sensitive to certain environmental pollutants, allowing them to function as effective and selective sensors for detecting heavy metals, pesticides, and persistent organic pollutants.

Therefore, the remarkable versatility, safety, and multifunctionality of CDs position them as powerful drivers of innovation in healthcare and environmental technologies. Continued research and development are expected to broaden their applications and enhance their societal impact, offering solutions to address some of global challenges.

References

[1] G. Gonçalves, Small, 20, 2311526 (2024)
[2] G. Gonçalves Nanoscale, 10, 12505 (2018)
[3] G. Gonçalves Nanoscale, 17,12579 (2025)

I10. ZnO Nanorods as Photocatalysts for the Degradation of Organic Pollutants in Water

Matejka Podlogar[1*], Tina Radošević[1], Martina Kocijan[2], Nik Gračanin[1],
Klara L. Konda[1], Daria J. Babić[2], Damjan Vengust[1], Slavko Bernik[1], Aleš Omerzu[2]
[1]Jožef Stefan Institute, Ljubljana, Slovenia
[2]University of Rijeka, Rijeka, Croatia
[*]matejka.podlogar@ijs.si

Environmental pollution, particularly the contamination of water systems with persistent organic compounds and microplastics, is urgent global challenge. Photocatalysis has emerged as a sustainable and effective method for degrading such pollutants, with zinc oxide (ZnO) as a promising photocatalyst due to its abundance, low cost, and environmental compatibility.

In our recent work, we focused on enhancing the photocatalytic performance of ZnO by tailoring its intrinsic properties. We investigated the natural evolution of defect populations during the solvothermal recrystallization of ZnO nanodots into nanorods at 150 and 200°C, as well as during low-temperature hydrothermal growth (90°C) of nanorod arrays from ZnO seed layers, followed by post-annealing treatments. The phase, structure and morphology of the resulting nanostructures were characterized using X-ray diffraction (XRD) and electron microscopy techniques (SEM, FIB-SEM, TEM). Defects were studied by Raman, photoluminescence (PL) and electron paramagnetic resonance (EPR) spectroscopy, and surface chemistry by X-ray photoelectron spectroscopy (XPS). These analyses were used to link structural and electronic properties to photocatalytic performance.

Our findings show that bulk defects, more than surface chemistry, play a significant role in pollutant degradation efficiency. Post-annealing processes of ZnO nanostructures influence their self-doping behavior and functional properties. This was demonstrated through the photocatalytic degradation of caffeine under simulated sunlight, used as a model contaminant. The results not only demonstrated high photocatalytic activity but also showed excellent stability and reusability. These characteristics highlight their strong potential for practical use in water purification and environmental remediation technologies.

References

[1] P. Seleš, M. Podlogar, *Et al. Ceramics International*, **50**, 26819 (2024).
[2] K.L. Konda, M. Podlogar, *Et al. under rewiew* (2025).

Topic: Micro / Nano Materials

I11. Stress effect on the structure of polycrystalline potassium sodium niobate piezoelectric thin films

Rui Pinho[1], **Oleksandr Tkach**[1, *], Rui Vialrinho[2], J. Agostinho Moreira[2],
Maxim Ivanov[1], M. Elisabete Costa[1], Paula M. Vilarinho[1]
[1]*CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Aveiro, Portugal*
[2]*IFIMUP, Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Department of Physics and Astronomy of Faculty of Sciences, University of Porto, Porto, Portugal*
[*] *Presenter's e-mail address: atkach@ua.pt*

Despite the piezoelectric market ruled by lead-based compounds there is a substantial literature on lead-free piezoelectrics. However, stress effects on the structural, dielectric, ferroelectric and piezoelectric performance of thin films have been barely addressed [1]. In this work, sol-gel derived $K_{0.5}Na_{0.5}NbO_3$ (KNN) films are deposited on platinized silicon (Pt/Si(100)), strontium titanate (Pt/STO(100)) and magnesium oxide (Pt/MgO(100)) substrates inducing stress of different sign and magnitude due to thermal expansion misfit. KNN films on Pt/Si are under tensile residual stress of +210 ± 28 MPa, while compressive residual stresses of -411 ± 18 MPa and -494 ± 26 MPa are found for KNN films on Pt/STO and Pt/MgO, respectively. While the film on Pt/Si with tensile residual stress shows the lowest room-temperature polarization with an almost neglected out-of-plane component of piezoresponse, compressive state promotes the increase of the dielectric permittivity, polarization and piezoresponse. Most important, transition temperatures are studied using variable-temperature Raman spectroscopy and found to be markedly affected by the type and magnitude of the residual stress. The highest transition temperatures and the widest temperature region for tetragonal phase are found for KNN films on Pt/Si. The lowest and the narrowest ones are recorded for KNN films on Pt/MgO. This work thus highlights the impact of stress as one of the key parameters in the performance of KNN polycrystalline thin films implying a possibility of the morphotropic phase boundary in KNN thin films under compressive residual stress [2].

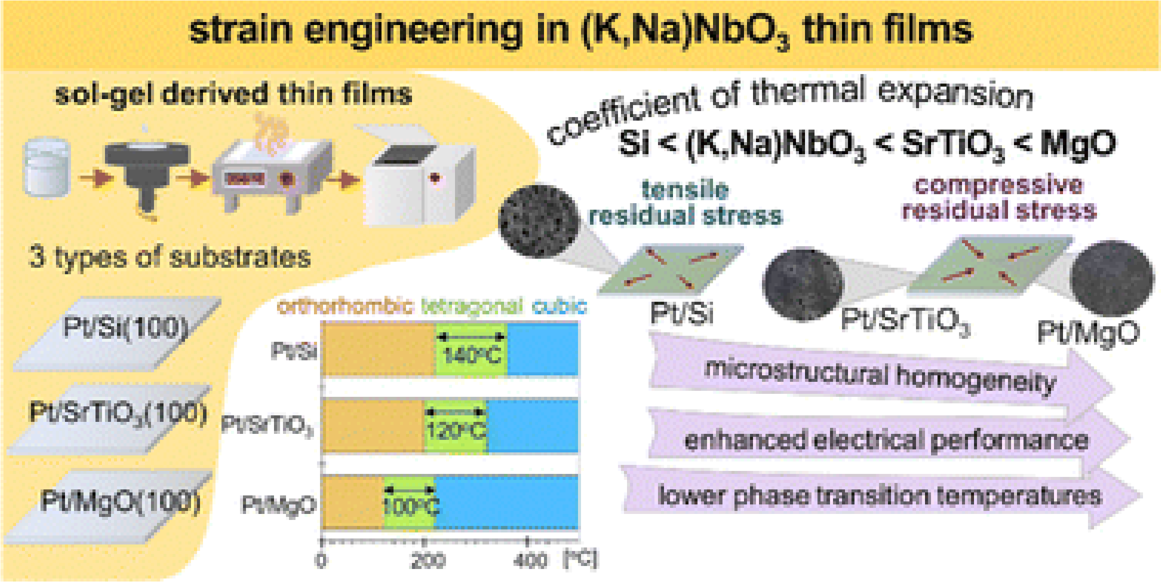


Figure 1. Graphical abstract.

References
[1] A. Tkach, et al., *Coatings* **8**, 449 (2018).
[2] R. Pinho, et al., *J. Mater. Chem. C* **23**, 7758 (2023).

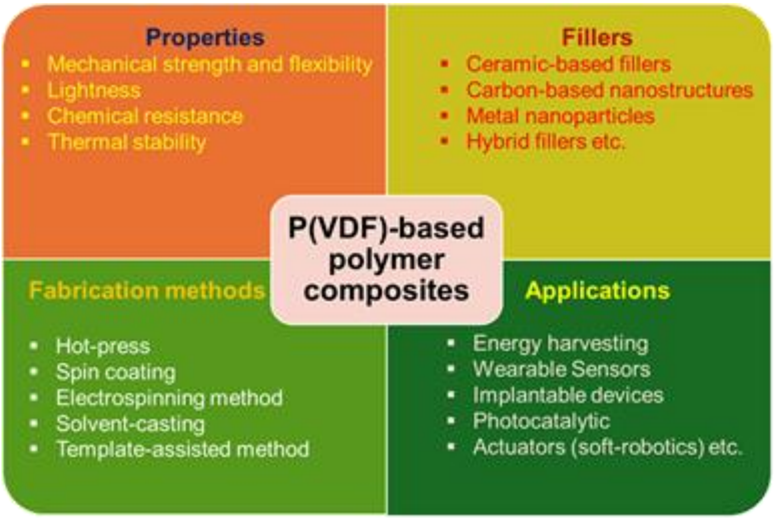
I12. PVDF-based polymer composites: A platform for multifarious applications

Indrani Coondoo[1,2 *]

[1]*Department of Materials and Ceramic Engineering, University of Aveiro, Portugal*
[2]*CICECO-Aveiro Institute of Materials, University of Aveiro, Portugal*
[*] *indrani.coondoo@ua.pt*

Poly(vinylidene fluoride) (PVDF) is a semi-crystalline fluoropolymer endowed with excellent chemical resistance, thermal stability, mechanical strength, and high dielectric constant [1]. Owing to its intrinsic piezoelectric, pyroelectric, and ferroelectric properties, PVDF-based composites capitalize on the good mechanical flexibility of the polymers and superior electrical properties of filler particles, have attracted increasing attention across various technological sectors. By incorporating functional fillers– such as ceramics, carbon-based nanomaterials, metallic nanoparticles, and organic dopants–into the PVDF matrix, researchers have been able to tailor and enhance the material's electrical, mechanical, and thermal properties. This capability makes PVDF-based composites a promising platform for multifarious applications spanning energy harvesting, sensing, actuation, filtration, biomedical engineering, and flexible electronics [2].

In energy-related applications, PVDF composites embedded with piezoelectric or dielectric fillers have shown exceptional promise in nanogenerators and capacitors, owing to enhanced energy conversion efficiency and dielectric performance.



Composites integrated with materials like $BaTiO_3$, ZnO, or graphene have demonstrated significantly improved piezoelectric coefficients, making them ideal candidates for self-powered wearable devices and smart textiles. Moreover, their electroactive properties make them suitable for use in electrocaloric and ferroelectric cooling systems [1].

In the realm of sensors and actuators, PVDF composites offer high sensitivity, flexibility, and durability. These materials are being increasingly utilized in tactile sensors, pressure sensors, and biomedical diagnostic tools. The ability of PVDF to transduce mechanical signals into electrical output (and vice versa) is greatly enhanced by filler-induced phase transitions from the α-phase to the β-phase, which possesses the highest piezoelectric response. This makes PVDF-based composites particularly advantageous for structural health monitoring and artificial skin technologies [1].

In biomedical fields, PVDF-based composites offer biocompatibility, making them suitable for implantable devices, tissue engineering scaffolds, and drug delivery systems. The piezoelectric nature of PVDF enables the stimulation of cellular activity, which is valuable in bone regeneration and neural interfaces. Additionally, the chemical inertness and processability of PVDF allow for custom-tailored biomedical devices that are both functional and safe [3].

The continued evolution of synthesis methods– such as electrospinning, solution casting, and additive manufacturing– has further enhanced the ability to fabricate PVDF composites with controlled morphology, dispersion, and functional architecture [2]. These advancements have opened new avenues for integrating PVDF-based composites into emerging technologies such as soft robotics, wearable electronics, and Internet of Things (IoT) devices.

In conclusion, PVDF-based polymer composites serve as a highly adaptable platform for a broad spectrum of applications, owing to their tunable properties and multifunctional nature. The ongoing research into material design, processing techniques, and novel fillers promises to unlock even more capabilities, consolidating PVDF’s role at the forefront of functional polymer composite materials.

References

[1] S. Sharma, S. S. Mishra, R. Kumar and R. M. Yadav, New J. Chem., 46, 18613 (2022).
[2] S. Mohammadpourfazeli, S. Arash, A. Ansari, S. Yang, K. Mallick and R. Bagherzadeh, RSC Adv., 13, 370 (2023).
[3] V. O. C. Concha, L. Timóteo , L. A. N. Duarte , J. O. Bahú, F. L. Munoz, A. P. Silva, L. Lodi, P. Severino, J. León-Pulido, and E. B. Souto, J. Mater. Sci. 59, 14185 (2024).

I13. Shifting the Action Spectrum of Azobenzene into the Red/NIR Region via Triplet-sensitization

Pankaj Bharmoria[1] *, Mila Miroshnichenko[1], Lukas Naimovičius[1],
Kasper Moth-Poulsen[1,2,3] *

[1] *Institute of Materials Science of Barcelona, ICMAB-CSIC, Bellaterra, Barcelona, 08193, Spain.*
[2] *Catalan Institution for Research & Advanced Studies, ICREA, Pg. Lluís Companys 23, Barcelona, Spain*
[3] *Department of Chemistry and Chemical Engineering, Chalmers University of Technology, Kemivagen 4, 412 96, Gothenburg, Sweden*
**Phone: +34-631190558, and e-mail address: pankajbharmoria@gmail.com; pbharmoria@icmab.es*

Abstract

Red and near-infrared photoswitchable drugs provide significant photo-pharmacological benefits due to the enhanced penetration of red/NIR through the skin. Conventionally such photoactivation is facilitated by mechanisms such as two- and three-photon absorption, excited-state absorption, and triplet-triplet annihilation upconversion, which necessitate higher photon fluences (W to kW cm-2) than the skin's resilience limit (200 mW cm^{-2}). We have developed a comprehensive method for the cis-to-trans photoisomerization of azobenzenes through triplet sensitization using Far-red and NIR-I illumination (730-850 nm) with a triplet photosensitizer, employing very low excitation powers.[1] This method is utilized to regulate the heart rate of a frog tadpole by means of cis-to-trans photoisomerization of an azobenzene-functionalized muscarinic acetylcholine receptor M2 agonist within the phototherapeutic window at low excitation powers.[2]

References

[1] P. Bharmoria, * S. Ghasemi, F. Edhborg, Kasper Moth-Poulsen, * et al. Chem. Sci. **13**, 11904-11911(2022).
[2] L. Naimovičius, M. Miroshnichenko, E. Opar, P. Bharmoria*, P. Gorostiza,* Kasper Moth-Poulsen.* et al. *Nat. Commun*. (2025), just accepted.

I14. A comparison of thermal and plasma-enhanced atomic layer deposition techniques of TiO_2 thin films for the photocatalytic degradation of pollutants from water

Martina Kocijan [1, *], Robert Peter [1,2], Iva Šarić Janković [1,2], Karlo Veličan [1,2],
Črtomir Donik [3], Ivna Kavre Piltaver [1,2]
[1]Faculty of Physics, University of Rijeka, Radmile Matejčić 2, 51 000 Rijeka, Croatia
[2]Center for Micro- and Nanosciences and Technologies, University of Rijeka,
Radmile Matejčić 2, 51 000 Rijeka, Croatia
[3] Institute of Metals and Technology, Lepi pot 11, 1000 Ljubljana, Slovenia
[*] martina.kocijan@uniri.hr

Global water demand has increased significantly due to population growth, economic development, and changing consumption patterns. These factors contribute to a growing problem by generating substantial amounts of wastewater. However, this wastewater represents a largely untapped resource for water recycling, which has the potential to reduce water stress and support a circular economy. The escalating global water crisis requires advanced wastewater treatment technologies that can effectively remove complex contaminants from water. Advanced oxidation processes (AOPs) provide promising and sustainable solutions for wastewater treatment [1]. Catalyst-based technologies, such as those utilising sunlight, have proven to be effective alternatives due to their lower energy consumption. However, the effectiveness of these technologies depends on innovations in the precise engineering of surface properties at the atomic level. Key properties for efficient photocatalysts include functionality, surface charge, and material durability. Thin films are crucial for various technologies, such as optoelectronic components, magnetic storage devices, and catalysts [2]. Vapour deposition methods, particularly atomic layer deposition (ALD), provide effective solutions for producing thin films on various substrates. ALD enables the preparation of nanoscale materials and provides exceptional control over surface, structure, and optical properties, thereby increasing the efficiency of wastewater treatment [3].

Thin films of titanium dioxide (TiO_2) have attracted considerable interest in recent years due to their unique properties applicable across a wide range of fields. The effective use of these remarkable functional properties depends primarily on the films' fundamental characteristics, such as structure and morphology, which are influenced by the deposition parameters. This research examines how thermal and plasma-enhanced atomic layer deposition (PEALD) conditions affect the structure and morphology of TiO_2 thin films deposited on Si (100). In the PEALD process, oxygen plasma is utilised as a co-reactant alongside titanium tetrachloride ($TiCl_4$), which serves as the metal precursor. The thermal ALD system employed water vapour as a co-reactant with the $TiCl_4$ precursor to deposit TiO_2 film. Detailed characterisation of TiO_2 films using scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), transmission electron microscopy (TEM), and UV–vis spectroscopy reveals how different synthesis techniques and temperatures impact their morphology, crystallisation, and optical properties. The photocatalytic activity of the synthesised TiO_2 films was examined in a cylindrical reactor equipped with a quartz cover. In this study, methylene blue (MB) was used as a model pollutant in deionised (DI) water. The solution was stirred while being exposed to a simulated solar spectrum generated by an Ultra Vitalux lamp (300 W, Osram) and UV irradiation from two 254 nm lamps (6 W, Osram). Research findings show that synthesis methods, such as thermal and PEALD, along with temperature variations, significantly influence the structure and surface morphology of TiO_2 thin films, which in turn influence their photocatalytic performance in degrading MB under both UV and solar irradiation.

Acknowledgment

The research leading to these results has received funding from the core funding NPOO.C3.2.R2-I1.06.0083 supported by the European Union NextGenerationEU.

References

[1] A. Jan, M.B. Tanis-Kanbur, L.C. Rietveld, and S.G.J. Heijman*, Open Ceramics*, **22**, 100780 (2025).
[2] S. Sakthinathan, G.A. Meenakshi, S. Vinothini, C.-L. Yu, C.-L. Chen, T.-W. Chiu, N. Vittayakorn, *Processes*, **13**, 587 (2025).
[3] T.-Y. Lee, P.-T. Chen, C.-C. Huang, H.-C. Chen, L.-Y. Chen, P.-T. Lee, F.-C. Chen, R.-H. Horng, H.-C Kuo, *Nanoscale Advances,* **7**, 2796-2817 (2025).

I15. Layered cobaltite electrodes for Protonic Ceramic Cells

Allan J. M. Araújo[1,2], Vanessa C. D. Graça, Rafael A. Raimundo[3], Antonio Lapenda[4], Daniel A. Macedo[4], **Francisco J. A. Loureiro**[1,2,*]

[1] TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.
[2] LASI - Intelligent Systems Associate Laboratory, 4800-058 Guimarães, Portugal.
[3] Department of Theoretical and Experimental Physics, UFRN – Federal University of Rio Grande do Norte, 59078-970 Natal, Brazil
[4] Materials Science and Engineering Postgraduate Program – PPCEM, Federal University of Paraíba – UFPB, 58051-900 João Pessoa, Brazil
* *francisco.loureiro@ua.pt.*

This study explores $Ba_2Co_9O_{14}$ (BCO), a layered cobaltite, as a potential oxygen electrode material for protonic ceramic cells (PCCs), which are promising clean energy devices operating at intermediate temperatures (400 – 700 °C). A key challenge in PCCs is improving the oxygen reduction reaction (ORR) at the cathode, which limits performance [1,2]. The unique layered structure of BCO compound, mixed cobalt oxidation states (Co^{2+}/Co^{3+}), and abundant surface oxygen vacancies are shown to enhance electrocatalytic activity. Structural and chemical analyses confirmed the purity, thermal stability, and suitable morphology of BCO for ORR. Additionally, electrochemical impedance spectroscopy (EIS) revealed low polarization resistance, comparable or superior to current state-of-the-art materials. The findings indicate that BCO is a chemically stable, efficient, and compatible electrode material for PCCs, supporting its potential use in advanced electrochemical energy conversion systems.

References

[1] C. Duan, R.J. Kee, H. Zhu, C. Karakaya, Y. Chen, S. Ricote, A. Jarry, E.J. Crumlin, D. Hook, R. Braun, N.P. Sullivan, R. O'Hayre, *Nature*, **557**, 217–222 (2018).
[2] A.J.M. Araújo, V.C.D. Graça, R.A. Raimundo, A.C.L. Filho, D.A. Macedo, F.J.A. Loureiro, A new layered barium cobaltite electrode for protonic ceramic cells, *J Mater Chem A*, **12**, 840–853 (2024).

Acknowledgements

The authors acknowledge the following grants/projects: COMPETE2030-FEDER-00820300, 2020.02797.CEECIND/CP1589/CT0030 (https://doi.org/10.54499/2020.02797.CEECIND/CP1589/CT0030), 2022.02498.PTDC (https://doi.org/10.54499/2022.02498.PTDC), UIDB/00481/2020 (https://doi.org/10.54499/UIDB/00481/2020), and UIDP/00481/2020 (https://doi.org/10.54499/UIDP/00481/2020) from Fundação para a Ciência e a Tecnologia (FCT). Rafael A. Raimundo and Daniel A. Macedo also acknowledge the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq/Brazil, 309430/2019-4 and 151879/2022-2). This study was also financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – Brasil (CAPES) – Finance Code 001.

I16. Exploring Multifunctionality: Optical, Impedance, and Photocatalytic Properties of $Dy_{0.5}Er_{0.5}CrO_3$ Nanomaterial

Neeraj Panwar*

Department of Physics, Chaudhary Charan Singh University Meerut-250004, Uttar Pradesh, India
***Email:** npanwar.phy@ccsuniversity.ac.in

The multifunctional properties, including optical, complex impedance, and photocatalytic performance of the $Dy_{0.5}Er_{0.5}CrO_3$ (DECO) compound fabricated via the sol-gel method, have been thoroughly investigated. The optical study revealed an optical bandgap energy of 2.67 eV, indicating its potential for solar-light-driven photocatalytic degradation of harmful organic dyes. The AC conductivity was investigated as a function of frequency and temperature. Its frequency dependence was found to follow Jonscher's power law. The temperature-dependent AC conductivity was explained by two models: the non-overlapping small polaron tunneling (NSPT) model and the correlated barrier hopping (CBH) model. The impedance data analysis revealed a non-Debye-type relaxation. The prepared material, in this study, demonstrated degradation efficiencies of 57% for Methylene Blue (MB) dye and 70% for Rhodamine B (RhB) dye.

I17. Artificial Intelligence (AI) Applications in Manufacturing

Musaab ZAROG

Department of Mechanical and Industrial Engineering, College of Engineering, Sultan Qaboos University, P.O. Box 33, Al-Khoudh, Muscat, 123, Sultanate of Oman

Intelligent manufacturing is an advanced production approach that utilizes Artificial Intelligence (AI), to create smart, responsive, and self-optimizing manufacturing environments. By enabling real-time data acquisition, autonomous decision-making, intelligent manufacturing systems significantly improve productivity, product quality, and resource efficiency. Among core components of AI application in manufacturing, predictive maintenance plays a critical role in ensuring equipment reliability, minimizing downtime, and optimizing operational efficiency. By leveraging real-time sensor data, machine learning algorithms, and historical maintenance records, predictive maintenance enables early fault detection and accurate forecasting of equipment failures. This paper explores the integration of intelligent manufacturing systems with predictive maintenance strategies, highlighting key technologies, implementation frameworks, and case studies from various industries. The synergy between intelligent automation and predictive analytics not only enhances productivity but also contributes to cost savings, safety, and sustainable manufacturing practices.

I18. Valorization of cork residues as adsorbents for water treatment

Carlos M. Granadeiro[1, *], Daniela S.S. Flores[1], João Mendes[1], Giovanna G.S. Grous[1], Paulo Macedo[2]
[1]LAQV-REQUIMTE, Department of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, 4169-007 Porto, Portugal
[2]J.A. Veiga de Macedo S.A., 4536-904 Santa Maria de Lamas, Portugal
[*] *cgranadeiro@fc.up.pt*

Cork, a renewable lignocellulosic material, is obtained from the bark of cork oak and its sustainable harvesting promotes regeneration without interfering in soil enrichment or carbon sequestration.[1] Cork industry generates a considerable amount of cork waste from the cork stopper manufacturing process, which is typically burned as source of energy.[2]. Recently, there has been an increasing interest in the preparation of waste-derived materials as alternative adsorbents due to its low cost, sustainability, wide availability of feedstocks and remarkable adsorptive capacities.[3]

We have explored the potential application of cork powder in the preparation of advanced magnetic adsorbents with enhanced adsorptive capabilities for water remediation. Two types of magnetic cork-derived composite materials were prepared following different synthetic methodologies. The first method involves the impregnation of previously synthesized magnetite nanoparticles into the porous framework of cork powder, while the second involves the impregnation of cork powder with a selected transition metal (Fe) followed by pyrolysis under inert atmosphere, leading to the formation of a magnetic biochar. The adsorptive ability of the magnetic cork-derived materials was evaluated for the removal of fluoroquinolone antibiotics, using levofloxacin as model molecule. The adsorption studies were carried out by fluorescence spectroscopy through monitoring of the fluorescent emission of levofloxacin. Optimization of the experimental parameters, namely initial pH, contact time, adsorbent loading, was performed and adsorption kinetics was studied. Both magnetic cork-derived adsorbents exhibited remarkable adsorptive capacities in short periods of time for the removal of levofloxacin from aqueous solutions. The proposed materials combine the low cost of the precursors, sustainable transformation of solid wastes into value-added products, easy magnetic separation and remarkable adsorptive performance highlighting its exceptional potential for application in water remediation.

References

[1] X. Zhang, I. Elsayed, R.M.O. Nayanathara, X. Song, R. Shmulsky and E.B. Hassan, *Journal of Environmental Chemical Engineering*, **10**, 107460 (2022).
[2] Y. Luo, J. Tao, Y. Shan, X. He, R. Peng, H. Wu, X. Xiao and X. Lu, *Journal of Energy Storage*, **77**, 109914 (2024).
[3] J. Gong, R. Liu, Y. Sun, J. Xu, M. Liang, Y. Sun, L. Long, *Industrial Crops and Products*, **208**, 117846 (2024).

I19. Portable desalinator using graphene oxide functionalized microporous membranes

Markus A.O. Porangaba, Niraldo M. M. Melo, Lucas T. Vila Nova
Marcos G. Ghislandi*
Engineering Campus (UACSA), Federal Rural University of Pernambuco (UFRPE), 54518-430 Cabo de Santo Agostinho, PE, Brazil
* *tel: 55 81 995414010, email: marcos.ghislandi@ufrpe.br*

This study focuses on the development of a low-cost, portable direct filtration system for brackish water desalination, utilizing functionalized microporous membranes. Commercial polyamide (PA) and mixed cellulose ester (MCE) membranes were coated with graphene oxide (GO) synthesized via a modified Hummers method and crosslinked with polyvinyl alcohol (PVA) and citric acid (CA). The functionalized membranes were integrated into an easy-to-assemble portable filtration unit, inspired by a syringe operation, and constructed using conventional plumbing materials.

Structural and morphological characterization of GO and the prepared membranes were performed using X-ray diffraction (XRD), Fourier Transform Infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). FTIR confirmed the presence of oxygenated groups typical of GO and the modified membranes, while XRD of crosslinked membranes showed traces of crystalline phases, possibly due to GO-PVA interactions. SEM images revealed that GO sheets were uniformly deposited on the PA membranes, forming a multilayer coat ranging from approximately 0.3 to 0.5 μm in thickness, depending on the amount of GO. The non-uniform surface structure of the pure polyamide membrane, with varied nano and micrometric pores, was also observed.

Mechanical stability tests using an ultrasonic bath demonstrated that PVA/CA reticulation significantly enhanced the mechanical stability of the membranes by promoting esterification crosslinking reactions between citric acid's carboxyl groups and the hydroxyl groups of PVA and GO. Non-crosslinked membranes (Method A) showed considerable loss of the deposited GO film after the ultrasound test compared to crosslinked membranes (Method B).

The membranes were evaluated for their salt rejection capacity against magnesium sulfate (MgSO4) and sodium chloride (NaCl) in aqueous solutions. Polyamide membranes consistently outperformed MCE membranes, attributed to the strong interaction between the carboxylic groups in GO and the amine groups in PA, enhancing chemical and mechanical stability. The PA0.75/RET membrane (polyamide modified with 0.75 mg of GO and crosslinked) exhibited the best performance, achieving 55% rejection and a permeability of 1.42 L/m2·h·bar for Mg+2 ions, and 37% rejection with a permeability of 2.08 L/m2·h·bar for Na+ ions. This superior rejection for divalent ions was linked to their larger charge/ionic radius ratio. The study proposes that electrostatic interactions and, predominantly, physical sieving are the main mechanisms for salt rejection.

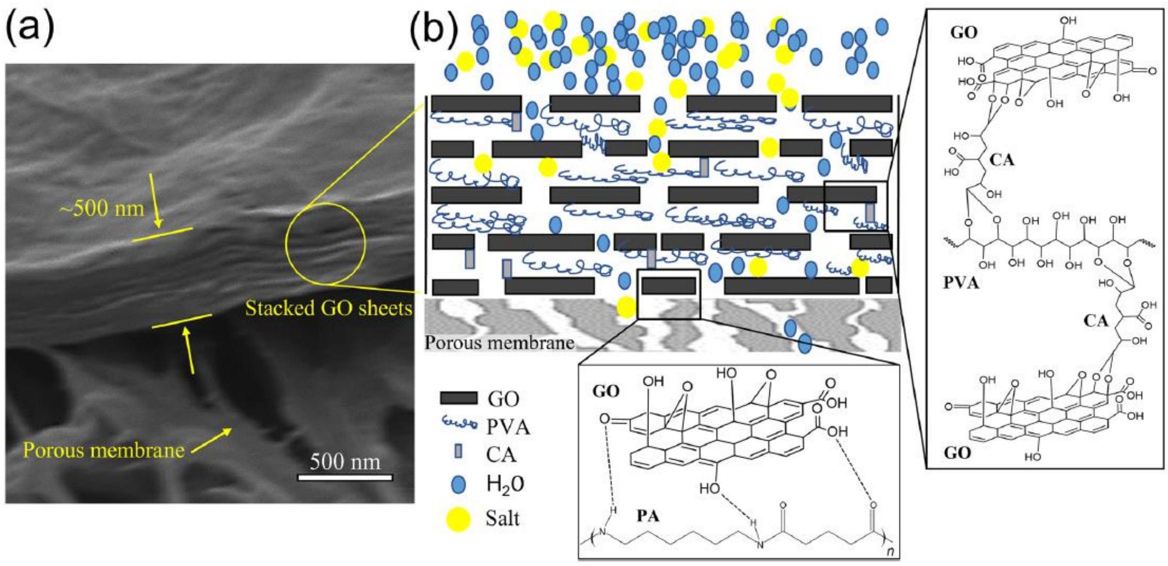


Fig. 1. (a) Coating of GO over the polyamide membrane: SEM showing the average thickness of GO layer, and (b) filtration mechanisms based on GO sheets with crosslinked polymer layers.

The modified membranes showed potential for reuse, maintaining over 29% retention for Mg+2 ions on the third reuse cycle. The increase in GO/PVA film thickness was observed to proportionally increase salt rejection while reducing permeability, indicating that the GO film acts as a pore-blocking agent. The assembled device proved stable at pressures of 4-5 bar and was found to be accurate and reproducible. These advancements highlight the practical potential for applying these functionalized membranes in portable desalination systems, as well as in other separation fields like post-treatment of brackish well water and wastewater.

References

[1] Sun, J., et al. J. Membr. Sci. **599**, 117838 (2020)
[2] Han, Y., Xu, Z., Gao, C., Adv. Funct. Mater. **23**, 3693–3700 (2013)
[3] M.A.O. Porangaba, R. A.A. Silva, D. F. Gomes, et al, Chem. Eng. Research and Design, **193**, 222-230, (2023)

I20. Vacancy diamond color centers process with machine learning

Jiang, Zhi[a]; Peres, Marco[b, c, d]; Gonçalves, Gil[a]
[a] *TEMA, Mechanical Engineering Department, University of Aveiro, Aveiro, 3810-193, Portugal*
[b] *Instituto de Engenharia de Sistemas e Computadores - Microssistemas e Nanotecnologia, Rua Alves Redol 9, 1000-029 Lisboa, Portugal*
[c] *IPFN, Instituto Superior Técnico, University of Lisbon, Av. Rovisco Pais 1, 1049 001 Lisbon, Portugal*
[d] *DECN, Instituto Superior Técnico, University of Lisbon, Estrada Nacional 10 (km 139.7), 2695 066 Bobadela, Portugal*

This article systematically reviews the key technologies and parameters involved in the synthesis of N-, Si-, Ge-, and Sn-vacancy color-center diamonds and presents a comprehensive analysis using machine learning (ML) approaches. We compared the distinctive characteristics and challenges of various synthesis and modification methods, including high-pressure high-temperature (HPHT) synthesis, microwave plasma chemical vapor deposition (MPCVD), ion implantation, and ion irradiation. By training specific parameters in the diamond growth environment, such as the annealing time, substrate temperature, and pressure, using extreme gradient boosting (XGB) and decision tree (DTR) models, the photoluminescence intensity and color-center concentration can be precisely predicted. The ML models successfully identified key output parameters (*e.g.*, size of HPHT vacancy centers, MPCVD plasma power, and annealing time after ion implantation or electron irradiation) to establish a close connection with the Debye-Waller factor (DWF), which indicates more coherent and efficient photon emission according to the optical efficiency of color centers and the zero-phonon line (ZPL) of photoluminescence.

We propose the use of machine learning to overcome these limitations. Our approach is based, specifically, on two ML methods: Extreme Gradient Boosting (XGB) and Decision Tree Regression (DTR).[1–3] Briefly, we performed an extensive metadata analysis of the existing literature (~60 studies and ~170 data sets 1) and created a large database containing the synthesis parameters and color centers yield for each one of the main diamond fabrication techniques. We then used this database to train and test the XGB and DTR algorithms and used this in combination with the Shapley value analysis to identify the optimal combination of synthesis parameters that produces ‘high-quality’ color centers. Note that here we use the Debye-Waller factor as proxy for the ‘quality’ of the VDCCs. This is motivated by a series of observations, specifically: i) the need to base our analysis on a measurable physical observable that is ii) common to all synthesis techniques, and iii) physically meaningful (many of the technological quantum realizations involving VDCCs heavily rely on their optical and spectral properties). The goal of this work is to provide a deterministic and practical guide for the optimization of diamond material synthesis and design for each synthesis protocol.

A total of 100 points from every PL spectrum of the retrieved literature were extracted, and the NV^-, SiV^-, GeV^-, and SnV^- VDCC values were calculated. The approximate number of VDCC studies and the distribution of DWF data are clearly shown by the violin plot in **Fig. 1**. According to the PL spectrum data of VDCCs,

$$I_{ZPL} = \int_{ZPL,range} I(\omega)d\omega, I_{total} = \int_{all,range} I(\omega)d\omega, DWF = \frac{I_{ZPL}}{I_{total}}$$

The ZPL peaks and all range of the entire emission spectra for every VDCCs were integrated, respectively. These DWF values indicate that VDCC centers have strong phonon coupling (small DWF), while SiV^-, GeV^-, SnV^- have much larger ZPL fractions (weaker phonon coupling).[4]

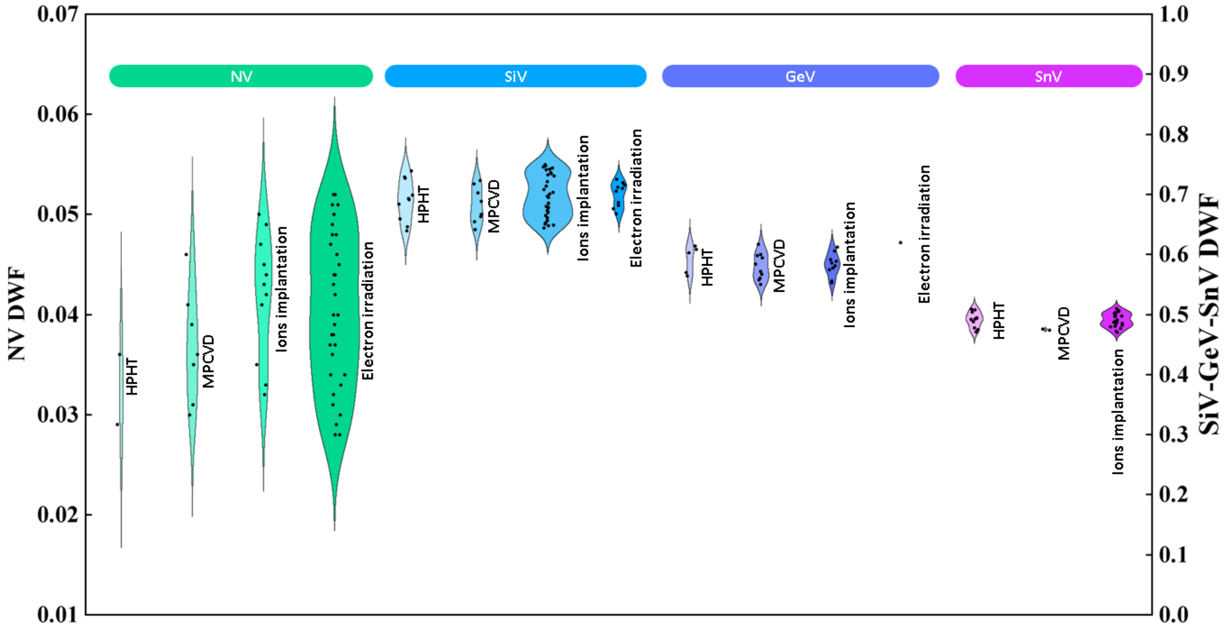


Figure 1. Debye-Waller factor (DWF) parameters of NV$^-$, SiV$^-$, GeV$^-$, and SnV$^-$, according to the ZPL intensity and total photoluminescence spectrum.

Acknowledgements

This research was funded by Horizon Europe (HORIZON), HORIZON-MSCA-2023- PF-01, under Grant101149632–GDSNL, and Fundação para a Ciência e a Tecnologia (FCT) trough the projects 10.54499/UIDB/00481/2020 (https://doi.org/10.54499/UIDB/00481/2020, and 10.54499/UIDP/00481/2020 (https://doi.org/10.54499/UIDP/00481/2020) and the project CarboNCT 2022.03596.PTDC (https://doi.org/10.54499/2022.03596.PTDC).

Reference

1. Poulsen, A. F. L. *et al.* Optimal control of a nitrogen-vacancy spin ensemble in diamond for sensing in the pulsed domain. *Physical Review B* **106**, 014202 (2022).
2. Choudhary, K. *et al.* Recent advances and applications of deep learning methods in materials science. *npj Computational Materials* **8**, 59 (2022).
3. Im, S. W. *et al.* Investigating chiral morphogenesis of gold using generative cellular automata. *Nature Materials* **23**, 977–983 (2024).
4. Lang, J. *et al.* Long optical coherence times of shallow-implanted, negatively charged silicon vacancy centers in diamond. *Applied Physics Letters* **116**, 064001 (2020).

I21. Tuneable, Printable, Injectable: Next-Gen Hydrogels for Functional Tissue Reconstruction

Fatma Ozdemir, Amelia Heslington, Kenny Dalgarno, Ana Ferreira Duarte, **Priscila Melo**

School of Engineering, Newcastle University. Newcastle Upon Tyne, United Kingdom

The development of hydrogels for tissue engineering and regenerative medicine has rapidly evolved to address the complex structural and functional demands of native tissues. This presentation focuses on recent advancements in hydrogel systems within Dr Melo's group, particularly collagen-based materials, tailored for mimicking and or regenerating cartilage and cardiac tissues. Collagen's inherent biocompatibility and structural similarity to the extracellular matrix make it a prime candidate for these applications. Innovations in click chemistry, including azide-alkyne reactions, have enabled the precise and efficient crosslinking of collagen networks, enhancing their mechanical stability and facilitating cell encapsulation within the scope of injectable therapies. For wound healing, chitosan-based hydrogels have emerged as promising platforms due to their antimicrobial properties, biodegradability, and ability to support angiogenesis. Additionally, composite hydrogels combining collagen and hyaluronic acid have shown great potential for modelling melanoma microenvironments and synovial tissues, offering tenable viscoelastic properties and cell-instructive cues. Notably, the majority of these hydrogel formulations are compatible with extrusion-based bioprinting and reactive jet impingement technologies, enabling the fabrication of anatomically relevant, cell-laden constructs and the possibility of creating multi-architecture constructs combining different biofabrication technologies. These developments underscore the critical role of hydrogel design and biofabrication techniques in advancing tissue engineering strategies for regenerative medicine and disease modelling.

I22. Porous Materials for Multimodal Micro-propulsion Systems for Small Spacecraft

M. Jugroot[1 *], P. Mallalieu[2], I. Savytskyy[3], G. Jones[4] and B. Little[5]

[1,2,3,4,5]*Mechanical and Aerospace Engineering, Royal Military College of Canada, Kingston, Canada*
[*]*RAPPEL Laboratory, Royal Military College of Canada, jugroot-m@rmc.ca*

Abstract

Smaller spacecraft, which have comparable capabilities to their larger predecessors, now comprise the majority of satellites launched into orbit. While satellites have scaled down in size, it has been a challenge to develop propulsion systems capable of operating in a low power regime with a small form factor. This challenge has led to most operational small satellites to omit a propulsion system. This research investigates micro propulsion technology which can be used to enhance the mission capabilities of small satellites. The porous materials used as emitters are crucial to the development and testing of a multimodal electrospray thrusters [1] which can operate either at higher thrust (force) or higher specific impulse (exhaust velocity). To characterize the multimodal microthruster, a diagnostic suite of experimental setup [2] were developed at the RMC Advanced Propulsion and Plasma Exploration Laboratory (RAPPEL Lab) [3]. The prototype thruster described in this research has demonstrated how various electrospray emitter fabrication methods of porous materials (and geometries) could be combined into a multimodal system while maintaining a small footprint: to provide either high exhaust velocity or effective thrust for small satellites.

References

[1] P. Mallalieu, M. Jugroot, *Journal of Electric Propulsion*, Nature-Springer, 2024.
[2] B. Little, M. Jugroot, *Vacuum*, Elsevier, 2019.
[3] B. Little, M. Jugroot, *Journal of Spacecraft and Rockets*, AIAA, 2020.

I23. Tailoring piezoelectrics for enhanced energy storage

E. Venkata Ramana*and M. A. Valente

I3N, Department of Physics, University of Aveiro, 3810-193, Aveiro, Portugal

Dielectric energy storage systems are distinguished by their rapid charge–discharge capabilities, high power density, and long cycle life, making them particularly suitable for advanced pulsed power systems and power conditioning applications. Their fast response and exceptional reliability are critical for emerging technologies such as electric vehicles, aerospace systems, and renewable energy integration.

Driven by the demand for high-performance dielectric materials, extensive research has focused on tuning ferroelectric properties through structural and compositional modifications. In this context, we explore the impact of induced relaxor behavior and composite formation on the energy storage performance of lead-free ferroelectric systems. By introducing compositional heterogeneity and local structural disorder, relaxor-like characteristics are activated—manifested by reversible domain switching and suppressed hysteresis losses. Concurrently, embedding secondary phases with tailored dielectric properties enhances the breakdown strength and boosts energy density, while maintaining high recoverable efficiency. Our findings reveal that the synergy between relaxor dynamics and composite engineering significantly enhances both energy density and efficiency. This work provides a promising pathway for the design of next-generation ferroelectric materials and offers valuable insights into the structure–property relationships underpinning advanced dielectric energy storage technologies.

References

[1] E.V. Ramana, A. Durairajan, D. Kavitha, D.M. Tobaldi, J. Zavašnik, I. Bdikin, M.A. Valente, J. Energy Storage 87 (2024) 111454

[2] Q. Chai, Z. Liu, Z. Deng, Z. Peng, X. Chao, J. Lu, H. Huang, S. Zhang, Z. Yang, Nature Commun. 16(1) (2025) 1633.

I24. Rare earth doped low phonon glasses for gas sensing

Suresh Kumar Jakka

i3N and Department of Physics, University of Aveiro, Aveiro, 3810-193, Portugal

Low phonon glasses such as tellurite or chalcaogenide doped with photoluminescent (PL) active ions, specially trivalent rare earth (RE^{3+}) ions offer significant advancements in gas sensing due to their enhanced optical properties and high sensitivity. The RE dopants impart distinct PL characteristics, enabling gas detection across visible (VIS), infrared (IR), and mid-infrared (MIR) regions. Each RE^{3+} ion has a distinct feature that could be used in sensing in various regions. For instance, Eu^{3+}-doped glasses, which emit sharply in the VIS around 615 nm, are ideal for detecting oxygen (O_2), as O_2 presence quenches PL intensity. Er^{3+}-doped glasses are effective in the IR region around 1.5 μm, suitable for carbon dioxide (CO_2) detection, with PL intensity correlating to CO_2 concentration. Yb^{3+}-doped tellurite glasses, emitting strongly in the MIR around 1 μm, are effective for sulfur dioxide (SO_2) detection, enhancing sensitivity and selectivity. Chalcogenide glasses doped with Er^{3+} and Yb^{3+} show potential for methane (CH_4) detection due to their broad MIR transmission and high refractive index. These glasses fabricated into optical fibers, can detect gases through changes in PL emission upon exposure. This method allows remote sensing, high sensitivity, and operation in harsh environments, making it suitable for environmental monitoring and industrial applications.

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

Acknowledgements: The author acknowledge FCT and FEDER funding agencies for the financial support in the form of the IC & DT project “ChalcoMethSensors”.

I25. Ellipsometric study of $\{Pb(Mg_{1/3}Nb_{2/3})O_3\}_{1-x}$ $\{PbTiO_3\}_x$: Evaluation of refractive index, extinction coefficient and optical band gap

Charul Joshi[1], Pratiksha Agnihotri[2], Radheshyam Rai[1*]
[1]School of Basic and applied sciences, Department of Physics, Galgotias University Greater Noida, Gautam Buddh Nagar, Uttar Pradesh-203201 India
[2]Ministry of Electronics and Information Technology, Electronics Niketan, 6, CGO Complex, New Delhi – 110003, India

This investigation delves into the analysis of the structural, microstructural, and optical characteristics of $\{Pb(Mg_{1/3}Nb_{2/3})\ O_3\}_{1-x}$ $\{PbTiO_3\}_x$ (x = 0.1, 0.2, 0.3, 0.4) prepared through the spin coating technique. The synthesized ceramics showed monoclinic structure which was verified by X-ray diffraction, showcasing distinct reflections that suggest a homogeneous composition. Examination of crystallite size and strain unveiled a pattern of initial growth, followed by reduction and subsequent increment, revealing intricate interactions between $PbTiO_3$ (PT) and $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN) lattice. Field emission scanning electron microscopic observations displayed fluctuations in particle dimensions, where a moderate PT content facilitated grain enlargement while higher concentrations impeded it. Through spectroscopic ellipsometry, it was illustrated that the refractive index and extinction coefficient underwent changes based on PT content, thereby influencing the optical characteristics. Initially, the band gap energy experienced an increase, with a subsequent slight decrease at higher PT concentrations. These results underscore the notable impact of PT content on the properties of the material, indicating its potential for customized optoelectronic applications.

I26. Exploiting strain gradients in biomaterials to conceptualize advanced bone grafts

Nathalie Barroca
Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Aveiro, Portugal
nbarroca@ua.pt

Tissue engineering often relies on scaffolds to create a microenvironment capable of harnessing cell's ability to repair damaged tissue. Instructive microenvironments have been developed by exploiting diverse biochemical and biophysical cues such as growth factors, exosomes, mechanical and electrical stimulation to guide cell adhesion, proliferation, and differentiation for effective regeneration.[1] In bone tissue, electrical stimulation may be particularly relevant since bone exhibits electromechanical properties, i.e. flexo- and piezoelectric properties. While collagen is piezoelectric and responds to homogeneous deformations, hydroxyapatite is flexoelectric and develops an electric field in response to inhomogeneous deformations.[2] When bending hydroxyapatite microcracks, large electric fields are generated and trigger bone cells to mineralize, suggesting a role in bone remodeling.[3] Since flexoelectricity is the property of all dielectric materials whereby they polarize when subjected to strain gradient, we questioned if inhomogeneous deformations could yield polarization in biomaterials, large enough to have relevance in bone repair applications. We experimentally evaluated the polarization in response to bending in biocompatible and biodegradable materials, well-established in both research and clinical settings. These are: bioactive glass 45S5, poly(L-Lactic acid) (PLLA), polycaprolactone (PCL) and their copolymers. Whereas PLLA, PCL and copolymers are widely used, they are also relatively inert and often require the incorporation of osteogenic additives such as hydroxyapatite. Thus, we also evaluated the bending-induced polarization in composites containing hydroxyapatite nanoparticles. A large range of flexoelectric response was observed and is discussed in terms of opportunities for customized scaffold designs for bone repair.

References

[1] G.L. Koons, M. Diba, A.G. Mikos, *Nat. Rev. Mater.* **5** 584–603 (2020).
[2] Abdollahi, D. Damjanovic, G. Catalan, *Adv. Mater.* **30** 1–5 (2018).
[3] R. Núñez-Toldrà, F. Vasquez-Sancho, N. Barroca, G. Catalan, *Sci. Rep.* **10** 1–10 (2020).

I27. Metal-Supported Proton-Conducting Electrochemical Cells: MnO_2 as a promising sintering additive

Vanessa C.D. Graça[1,2]*, Geraud Stoven[3], Laura I.V.Holz [1,2], Francisco J.A. Loureiro [1,2], Duncan P.Fagg [1,2]
[1] *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.*
[2] *LASI - Intelligent Systems Associate Laboratory, Portugal.*
[3] *University of Tours, France*
* *vanessagraca@ua.pt*

A new category of ceramic electrochemical devices, referred to as metal-supported protonic ceramic electrochemical cells (MS-PCECs), is attracting attention due to their combination of the outstanding mechanical characteristics of metal supports and the high efficiency coupled with low-temperature operation of proton-conducting ceramics, allowing them to operate effectively in challenging conditions, particularly those involving high pressure or rapid temperature changes [1].

Nevertheless, several significant challenges have been recognized in the fabrication of these structures, such as issues with chemical compatibility, incomplete sintering of the electrolyte, and the loss of barium-based materials during electrolyte densification. To tackle these challenges, lowering the sintering temperature may prove advantageous by incorporating sintering additives [1,2]. However, there is currently limited information available regarding potential additives since these devices need to be produced under reducing environments to prevent the metal support from oxidizing. Thus, this study evaluates the effect of incorporating small quantities of MnO_2 on the sintering behaviour of the electrolyte material $BaCe_{0.4}Zr_{0.4}Y_{0.2}O_3$ (BCZY44) under reducing conditions.

A variety of characterisation methods, including X-ray diffraction (XRD), scanning electron microscopy/energy dispersive spectroscopy (SEM/EDS), dilatometry, and impedance spectroscopy (IES), are employed to analyze the processed materials.

Our results reveal that the addition of MnO2 enhances the sinterability of the BCZY44 electrolyte in reducing conditions, leading to increased grain growth and a decrease in the densification temperature, as observed through dilatometry and microstructural examinations. Additionally, the influence of MnO2 on the resultant conductivity of the electrolyte was investigated based on its concentration, using IES conducted under controlled temperature and humidity conditions, to determine whether the inclusion of this sintering additive affected the levels of protonic conductivity.

In summary, this work establishes the foundation necessary to evaluate the utility of MnO2 as a potential sintering aid for developing low-temperature MS-PCEC cells; research that may unlock their potential as durable electrochemical devices capable of operating in complex application environments.

The authors acknowledge the grants/projects with references: 2023.05868.CEECIND (https://doi.org/10.54499/2023.05868.CEECIND/CP2840/CT0021) ,2020.02797.CEECIND/CP1589/CT0030 (https://doi.org/10.54499/2020.02797.CEECIND/CP1589/CT0030), 2022.09319.PTDC (https://doi.org/10.54499/2022.09319.PTDC), 2022.02498.PTDC (https://doi.org/10.54499/2022.02498.PTDC), UIDB/00481/2020 (https://doi.org/10.54499/UIDB/00481/2020), and 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), and the projects COMPETE2030-FEDER-00744500 16284 2023.17866.ICDT, COMPETE2030-FEDER-00770000 16527 2023.17134.ICDT and COMPETE2030-FEDER-00820300 16919 2023.18516.ICDT.

References

[1] R. Wang et al. Int. J. Hydrogen Energy, vol. 44, nº 26, pp. 13768–13776, 2019 . https://doi.org/10.1016/j.ijhydene.2019.03.181

[2] G. Y. Lau, M. C. Tucker, ECS Meeting Abstracts, vol. MA2021-03, p. 83, 2021. https://doi.org/10.1149/MA2021-03183mtgabs

I28. Modern Approaches of Energy Storage through Magnesium Hydride for Vehicular Applications

D. Pukazhselvan* [1,2] and Duncan Paul Fagg[1,2]
[1]*Department of Mechanical Engineering, TEMA - Centre for Mechanical Technology and Automation, University of Aveiro, Aveiro 3810-193, Portugal*
[2]*LASI - Intelligent Systems Associate Laboratory, Guimarães 4800-058, Portugal* *
**Email: dpukazh@ua.pt*

INTRODUCTION

Hydrogen is widely recognized as a clean and sustainable energy carrier due to its high gravimetric energy density and the carbon free energy delivery. However, the widespread adoption of hydrogen technologies is constrained by the challenge of storing hydrogen with high gravimetric/volumetric energy density. Solid-state hydrogen storage materials offer a promising solution, providing safer, more compact, and reversible storage under moderate operating conditions. Among the several lightweight metal hydride systems investigated over time, magnesium hydride (MgH_2) is a standout candidate owing to its high theoretical hydrogen storage capacity (~7.6 wt.%), low cost, natural abundance, and environmental benignity (USDOE target for vehicular applications: 5.5 to 6.5 wt.% H_2) [1]. Despite its advantages, MgH_2 suffers from intrinsically slow hydrogen absorption and desorption kinetics and requires high temperatures (>300 °C) for hydrogen release, limiting its practical application. To address these issues, in our laboratory we have recently optimized the synthesis of research grade MgH_2 (99.9%) and catalytically elevated the synthesized MgH_2 through the incorporation of metal oxide additives. Nanoconfinement approaches were employed, which makes the material durable with the powder quality maintained without getting influenced by aging factors. New research lines are developed, for example reactive hydride composites (RHC) and integration of metal hydride systems (typically, MgH_2 as anode active material) with Li ion batteries. These developments underscore the versatility of MgH_2 and its potential as a multifunctional material in the evolving landscape of energy storage.

EXPERIMENTAL

Additives (typically 5 wt.%) were incorporated with MgH_2 through mechanical milling using a Retsch PM 200 ball mill. Milling was conducted at a ball-to-powder weight ratio of 1:70, with a speed of 200-350 rpm for 5 hours. Hydrogen storage measurements were performed by Sieverts volumetric technique. The structural and chemical characteristics were analyzed through X-ray diffraction (XRD), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), differential scanning calorimetry (DSC), and Raman/infrared (IR) spectroscopy.

RESULTS AND DISCUSSION

Our approaches [2], including high-purity synthesis, catalytic enhancement with metal oxides, and nanoconfinement strategies, enabled MgH_2 to reversibly store approximately 6 wt.% hydrogen within a temperature range of 200–300 °C, achieving full hydrogenation in 5 to 10 minutes. Mechanistic studies revealed that the functional metal oxides (e.g., TiO_2, V_2O_5 and Nb_2O_5) chemically interact with MgH_2 and make catalytically active in-situ products typified by a formula unit $Mg_xM_yO_{x+y}$ (M= Ti, Nb, V), which promotes the release and restoration of hydrogen by lowering the temperature by at least 100 °C. Furthermore, MgH_2 forms reactive hydride composites (RHCs) with $LiBH_4$, which allow us the reuse of $LiBH_4$ and provide a hydrogen storage capacity >10 wt.%, surpassing USDOE targets. Additionally, MgH_2 demonstrates promise as an anode active material for lithium-ion batteries, delivering a theoretical capacity of ~2037 mAh/g (experimentally 1000 to 1500 mAh/g), significantly higher than conventional graphite anodes.

CONCLUSION

The advancements in synthesis, catalysis, and composite formation reaffirm MgH_2 as a multifunctional material with significant potential for hydrogen and electrochemical energy storage applications. These developments contribute to meeting DOE targets and open exciting pathways for further innovation in sustainable energy storage technologies. The future of MgH_2 based systems is bright with many new opportunities emerging for scientific and technological growth across the globe.

REFERENCES

1. USDOE, Target explanation document: onboard hydrogen storage for light-duty fuel cell vehicles, USDRIVE (2017), pp. 1-19
2. D. Pukazhselvan et al. Nanomaterials for Sustainable energy and environmental Remediation, Elsevier (2020), pp. 97-163.

ACKNOWLEDGMENTS

This article was supported by the projects UIDB/00481/2020 and UIDP/00481/2020 - Fundação para a Ciência e a Tecnologia, DOI 10.54499/UIDB/00481/2020 (https://doi.org/10.54499/UIDB/00481/2020) and DOI 10.54499/UIDP/00481/2020 (https://doi.org/10.54499/UIDP/00481/2020). D. P acknowledges FCT, Portugal for the financial support with reference CEECIND/04158/2017.

I29. Exploring transition metal nitrides as anode for ammonia solid oxide fuel cells

Laura I.V.Holz [1,2 *], Vanessa C.D. Graça [1,2], Francisco J.A. Loureiro [1,2],
Sergey M. Mikhalev [1,2], Duncan P.Fagg [1,2]

[1] *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.*
[2] *LASI - Intelligent Systems Associate Laboratory, Portugal.*
*lauraholz@ua.pt

Although ammonia (NH_3) is showing promise as an energy carrier for solid oxide fuel cells (SOFCs), finding substitute anode materials that provide improved performance, stability, and durability is still difficult [1–2]. In light of this, we have created a new anode composite that uses 8 mol% yttria-stabilized zirconia (8YSZ) as the oxide ion conducting phase and vanadium oxynitride (VON) as the electronic conducting phase. This anode was thoroughly characterized using several techniques, including X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Thermogravimetric Analysis (TGA), and Electrochemical Impedance Spectroscopy (EIS).

The findings showed that VON and 8YSZ had good chemical compatibility at high temperatures (1150 °C) and under reducing conditions (10%H_2 –90%N_2). With only slight mass changes attributable to changes in the nitrogen-to-oxygen ratio, TGA analysis verified the thermal stability of VON under these conditions. EIS was used to examine the anode's electrochemical behavior in an ammonia atmosphere over a temperature range of 650 to 800 °C. The electrode mechanism that was observed was similar to that of traditional Ni-based ceramics that function in hydrogen environments. Notably, the ammonia flow rate had a significant impact on the polarization resistance, which increased at higher flow rates as a result of limitations in gas conversion and diffusion.

As far as we know, this is the first study to describe using vanadium oxynitride as an anode material for ammonia-SOFCs.

References

[1] R. Lan and S. Tao, Front. Energy Res., 2014, **2**, 1–4 .

[2] J. Yang, A. F. S. Molouk, T. Okanishi, H. Muroyama, T. Matsui and K. Eguchi, ACS Appl. Mater. Interfaces, 2015, **7**, 28701– 28707.

Exploring transition metal nitrides as anode for ammonia solid oxide fuel cells

Laura I.V.Holz [1,2] *, Vanessa C.D. Graça [1,2], Francisco J.A. Loureiro [1,2],
Sergey M. Mikhalev[1,2], Duncan P.Fagg [1,2]
[1] *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.*
[2] *LASI - Intelligent Systems Associate Laboratory, Portugal.*
* lauraholz@ua.pt

Although ammonia (NH_3) is showing promise as an energy carrier for solid oxide fuel cells (SOFCs), finding substitute anode materials that provide improved performance, stability, and durability is still difficult [1–2]. In light of this, we have created a new anode composite that uses 8 mol% yttria-stabilized zirconia (8YSZ) as the oxide ion conducting phase and vanadium oxynitride (VON) as the electronic conducting phase. This anode was thoroughly characterized using several techniques, including X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Thermogravimetric Analysis (TGA), and Electrochemical Impedance Spectroscopy (EIS).

The findings showed that VON and 8YSZ had good chemical compatibility at high temperatures (1150 °C) and under reducing conditions (10%H_2 –90%N_2). With only slight mass changes attributable to changes in the nitrogen-to-oxygen ratio, TGA analysis verified the thermal stability of VON under these conditions. EIS was used to examine the anode's electrochemical behavior in an ammonia atmosphere over a temperature range of 650 to 800 °C. The electrode mechanism that was observed was similar to that of traditional Ni-based ceramics that function in hydrogen environments. Notably, the ammonia flow rate had a significant impact on the polarization resistance, which increased at higher flow rates as a result of limitations in gas conversion and diffusion.

As far as we know, this is the first study to describe using vanadium oxynitride as an anode material for ammonia-SOFCs.

Acknowledgements

The authors acknowledge the grants/projects with references: 2023.05868.CEECIND (https://doi.org/10.54499/2023.05868.CEECIND/CP2840/CT0021) ,2020.02797.CEECIND/CP1589/ CT0030 (https://doi.org/10.54499/2020.02797.CEECIND/CP1589/CT0030), 2022.09319.PTDC (https://doi.org/10.54499/2022.09319.PTDC), 2022.02498.PTDC (https://doi.org/10.54499/2022.02498.PTDC), UIDB/00481/2020 (https://doi.org/10.54499/UIDB/00481/2020), and 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), and the projects COMPETE2030-FEDER-00744500 16284 2023.17866.ICDT, COMPETE2030-FEDER-00770000 16527 2023.17134.ICDT and COMPETE2030-FEDER-00820300 16919 2023.18516.ICDT.

References

[1] R. Lan and S. Tao, Front. Energy Res., 2014, **2**, 1–4 .
[2] J. Yang, A. F. S. Molouk, T. Okanishi, H. Muroyama, T. Matsui and K. Eguchi, ACS Appl. Mater. Interfaces, 2015, **7**, 28701– 28707.

Oral presentations

O1. Synthesis, Characterization of $Pr(OH)_3$ -PQ Nano-Composite for Enhanced Photocatalytic Activities

Ganesh P. Jadhav, Vikram U. Pandit*

Haribhai V. Desai College of Arts, Science and Commerce (Autonomous) Pune, India

* vikramupandit@gmail.com

In the current work, an efficient Hydrothermal technique was used to develop a new $Pr(OH)_3$-PQ Nano-Composite in which ratio of PQ is 1% 5% & 10% Respectively. Fourier Transform Infrared Spectroscopy (FTIR), X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), (UV-DRS) Ultraviolet-Visible Diffuse Reflectance Spectroscopy and Energy Dispersive X-ray (EDX) were used for vibrational, structural, morphological, band gap and compositional analysis. The photocatalytic activity of nanocomposite was assessed against organic dye pollutant Rhodamine 6G under the sunlight irradiation and Photocatalytic Reactor. The enhanced photocatalytic activities can be attributed to the presence of higher percentage of active crystal facet (100), higher concentration of defects densities and narrower band gap. Thus, $Pr(OH)_3$ nanowires can be considered as a potential candidate for the application of wastewater treatment and related technologies.

O2. Developing 3D Aerogel from Magnetized Graphene Oxide and Biomass-derived Cellulose for Effective Antibiotics Removal

Lam-Tuan-Cuong Dang[1,2], Van-Kieu Nguyen[3,4], Le-Thuy-Thuy-Trang Hoang[1,2,*]
[1]*Laboratory of Advanced Materials Chemistry, Institute for Advanced Study in Technology, Ton Duc Thang University, Ho Chi Minh City, Vietnam*
[2]*Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Vietnam*
[3]*Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh, Vietnam*
[4]*Faculty of Natural Sciences, Duy Tan University, Da Nang 550000, Vietnam*
Tel.:(+84)792159952; E-mail: danglamtuancuong@tdtu.edu.vn

Abstract

In this study, a magnetized graphene oxide/banana peel-derived cellulose (M-GO/bio-cellulose) aerogel was successfully synthesized using ultrasound-assisted mechanical mixing technique and freeze-drying method. Characterization results confirmed the formation of the M-GO/bio-cellulose aerogel with the uniform scattering of Fe_3O_4 on the GO sheets embedded in the bio-cellulose scaffolds. Adsorption kinetic and isotherm studies suggested that experimental data fitted well the Elovich and the Sips models, respectively, with a maximum adsorption capacity of 238.7 mg g^{-1}. Freundlich isotherm model indicated the favorable multilayer adsorption of tetracycline onto the heterogeneous surface of the adsorbent. The obtained results showed the promising potential of M-GO/bio-cellulose aerogel for the high-performance adsorption of tetracycline.

Introduction

Tetracycline (TC), a commonly used antibiotic, is frequently detected in water sources due to its widespread use and incomplete metabolism in humans and animals [1]. Its persistence in the environment poses risks to aquatic life and public health. Among various treatment methods, adsorption is considered efficient and economical for removing such pollutants from water [2]. GO-based composite aerogels are promising adsorbents due to their large surface area and functional groups [3]. The M-GO/bio-cellulose aerogel was integrated into an eco-friendly and cost-effective biosorbent for high-performance TC removal.

Method

GO was synthesized using modified Hummers' method, attached Fe_3O_4 nanoparticles on the surface to produce M-GO. Cellulose isolated from banana peels using alkali and acid treatments. The aerogel was fabricated by ultrasonic dispersion of these components, followed by freeze-drying. FTIR spectra, Raman spectra, XRD patterns, FE-SEM images, EDX spectrum, and VSM analysis were used for material characterization. Batch adsorption tests examined the effects of solution pH, adsorbent dose, contact time, and initial TC concentration on the adsorption performance.

Results and discussion

FTIR, Raman, and XRD analyses confirmed the successful incorporation of GO, Fe_3O_4, and cellulose into the aerogel. FE-SEM images showed a porous, interconnected structure with dispersed Fe_3O_4 particles, supported by EDX mapping. VSM analysis revealed superparamagnetic behavior, facilitating the post-use magnetic separation of the biosorbent. Adsorption studies showed the highest capacity at pH 5.0 due to electrostatic attraction between the negatively charged aerogel and zwitterionic TC. Above pH 6, capacity declined due to repulsion with anionic TC. Lower doses achieved greater adsorption capacity. Kinetic data fitted well with the Elovich model, suggesting chemisorption on a heterogeneous surface. Adsorption isotherm analysis revealed that the Sips and Freundlich models were the best representation of the experimental data, indicating multilayer adsorption with diverse site energies. The maximum adsorption capacity (q_m) reached 238.7 mg g^{-1}, outperforming many bio-based adsorbents. FTIR spectra and XRD data post-adsorption indicated no structural collapse and confirmed interactions such as π–π stacking, hydrogen bonding, and electrostatic attraction. In a nutshell, these results support a multi-mechanistic model involving surface adsorption, pore-filling, and specific functional group interactions.

References

[1] Yingjie Dai, Mei Liu, Jingjing Li, Shengshu Yang, Yue Sun, Qiya Sun, Wensi Wang, Lu Lu, Kexin Zhang, Jiayi Xu, Wenlei Zheng, Zhaoyue Hu, Yahan Yang, Yuewen Gao, and Zhihua Liu, *Separation science and technology,* **55**, 1005-1021 (2020).

[2] Maryam Beiranvand, Saeed Farhadi, and Abdolnasar Mohammadi-Gholami, *RSC advances,* **12**, 34438-34453 (2022).

[3] Lucas Lentz, Diego Alex Mayer, Mirelle Dogenski, and Sandra Regina Salvador Ferreira, *Materials Chemistry and Physics,* **283**, 125981 (2022).

O3. Molecular dynamics simulation of Titanium Carbide MXene/Graphene heterostructure

Rahele Moghaddam [*], **Jamal Davoodi** [*], Neda Mousavi
Department of Physics, Faculty of science, University of Zanjan, Zanjan, Iran
[*] *+989123410391, +982433052353, jdavoodi@znu.ac.ir*

Recently, a large family of two dimensional transition metal carbides and nitrides, called MXenes [1], become interest due to their important applications [2], such as Li ion batteries, electrocatalysis and supercapacitors. MXenes have a public formula of Mn+1XnTx (n=1, 2 or 3), which M is early transition metal (i.e. Ti. Nb, V, Mo), X is carbon or nitrogen and Tx shows surface functional termination, such as –OH, -O, or –F. Stacking two dimensional material, such as graphene and MXene, which called heterostructure [3], provides novel properties to use at nanoelectronic. The aim of our research is to study the MXene/graphene heterostructure to the hope of obtaining new favorites properties. In the current study, we used molecular dynamics (MD) simulation technique to investigate mechanical properties of MXene, graphene as well as MXene/graphene heterostructure. The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package used to do molecular dynamics simulation. The Nose-Hover thermostat was applied for temperature control. Also, we used the periodic boundary condition in order to control the number of atoms. The stress-strain diagram obtained from our MD simulation using tensile tests. The mechanical properties, such as Young's modulus, fracture strength, failure strain and tensile strength of MXene/graphene heterostructure were obtained by the stress-strain diagram. Our results shown that the graphene present has remarkable effect on the mechanical properties.

References

[1] M. Naguib, et al., *Advanced Materials*, **23**, 4248-53 (2011).
[2] Y. Li, et al, *ACS Applied Nano Materials*, **4**, 5058-5067 (2021).

O4. Synergistic Composite Adsorbents for Advanced Radioactive Decontamination and Environmental Safety

FALAH Fatima Zahra[1,2 *], EL. GHAILASSI Touria[2], BOUAMRANI Mouna Latifa[1], HAMDANE Hasna[2], MOUSSAIF Ahmed[2], YOUSFI Samia[1]

[1]Laboratory of Analytical and Molecular Chemistry, Faculty of Sciences Ben M'Sick, Hassan II University of Casablanca, Morocco.

[2]National Center of Science, Technology and Nuclear Energy (CNESTEN), Morocco; Center for Nuclear Maamoura (CENM), Rabat, Morocco

[*] +212-619483413, fz.falah9@gmail.com

In the quest for effective radioactive decontamination solutions, composite materials have emerged as powerful adsorbents capable of targeting and immobilizing hazardous contaminants [1]. This study presents a novel bio-composite adsorbent designed to enhance the removal efficiency of radioactive ions from aqueous environments, promoting both environmental safety and sustainable remediation. By integrating chitosan with high-affinity cross-linkers, we achieve a synergistic effect that significantly improves adsorptive interactions and material stability under diverse conditions.

Through comprehensive isotherm, kinetic, and thermodynamic analyses, we explore the adsorption mechanisms and binding capacities of these composites, highlighting their superior performance compared to conventional materials. Further optimization using Box-Behnken design enables precise tuning of adsorption parameters, allowing the composite to effectively target specific radionuclides. This approach demonstrates the potential of these eco-friendly composite adsorbents as scalable and cost-effective solutions for advanced radioactive waste treatment, contributing to safer and cleaner water resources.

References

[1] de Araujo, L. G., Medeiros, V. L., de Paula Guarnieri, G., da Silva, D. A., Watanabe, T., Marumo, J. T., & Nery, J. G. Environmental Science: Advances, 2(3), 484-494 (2023).

O5. Hydrodynamics of Electron-hole Coulomb Drag

Yu. A. Pusep[1,*], M. A. T. Patricio[1], G. M. Jacobsen[2], M. D. Teodoro[2], G. M. Gusev[3], A. K. Bakarov[3]

[1]São Carlos Institute of Physics, University of São Paulo, 13560-970 São Carlos, SP, Brazil.
[2]Physics Department, Federal University of São Carlos, 13565-905, São Carlos, SP, Brazil.
[3]Institute of Physics, University of São Paulo, 135960-170 São Paulo, SP, Brazil.
**+55-16-34110572, pusep@ifsc.usp.br*

We study the transport of holes photoinjected into a mesoscopic GaAs channel made of a high-mobility GaAs/AlGaAs quantum well, where electrons exhibit hydrodynamic properties. A microscopic image of the sample is shown in Fig.1(a). A constant electric field applied to the collecting probes 3 and 4 leads to a corresponding DC electric current I_{34}. Laser excitation causes injection of holes from the barriers into the channel, which diffuse from the laser spot to collecting probes 3 and 4, where they recombine with background electrons, reducing the current I_{34}.

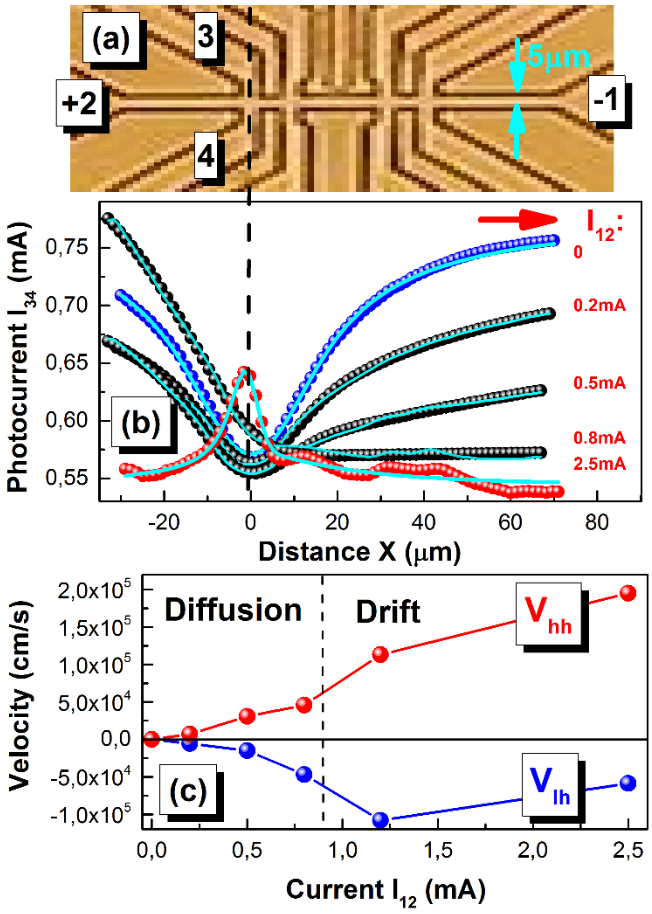


Fig.1. (a) Microscope image of the sample, (b) photocurrent I_{34} (circles) measured at T=3.7K between the collecting probes 3 and 4 at different electric currents I_{12} through the probes 1 and 2. The cyan lines represent calculated spatial diffusion profiles. Red arrow indicates the direction of electric current, (c) effective drift velocity of holes obtained by fitting the diffusion profiles in (a).

This current I_{34}, measured as a function of the distance X between the laser spot and the collection probes, reproduces the spatial diffusion profile of the holes shown in Fig.1(b), which is composed by superposition of the diffusion profiles of light and heavy holes. An external electric field applied to the channel creates a corresponding current I_{12} and leads to an increase in the effective diffusion length of holes. It was found that the effective length of heavy holes increases due to their drift, while the increase in the effective length of light holes is due to their Coulomb drag by electrons. As a result of the different actions of an external electric field on light and heavy holes, a remarkable effect was discovered in which an external electric field causes counter flows of heavy and light holes, demonstrated in Fig.1(c): heavy holes propagate in the direction of the electric field ($V_{hh} > 0$), while light holes move in the direction opposite to the electric field ($V_{lh} < 0$), in the same direction as the electrons. As a consequence of the Coulomb electron-hole drag, negative conductivity of light holes is observed. Moreover, an increase in the effective diffusion length of holes leads to a change in their transport regime from diffusion to drift, when the diffusion length exceeds the channel length. A theoretical model of the Coulomb drag of holes by electrons is developed, which made it possible to determine the characteristic parameters of the hydrodynamic electron-hole system such as diffusion coefficients, effective drift velocities and effective diffusion lengths of light and heavy holes. The theory explains well the obtained experimental results. The cardinal help of M.M. Glazov in substantiating the theory is acknowledged.

O6. Enhanced Corrosion and Wear Resistance of Nickel Coatings on Copper in NaCl Media via the Integration of Synthesized Graphene Nanosheets by electrochemical exfoliation into the Nickel Matrix

Amira Gharbi *, Youcef Hamlaoui

Laboratory of Physics of Matter and Radiation (LPMR), Faculty of Science and Technology, University Mohamed Cherif Messaadia, BP 1553-41000 Souk Ahras, Algeria

* *+213553142948, amira.gharbi@univ-soukahras.dz*

The present study focuses on graphene nanosheets synthesis via electrochemical exfoliation and its integration into the nickel matrix on developing Ni-graphene composite coatings via electrodeposition to enhance the corrosion resistance of nickel coatings on copper substrates in a 0.5 M NaCl solution. The composite coatings were fabricated using chronopotentiometry (Cp) at a current density of 50 mA/cm² for 10 minutes at 55°C, ensuring uniform dispersion of graphene within the Ni matrix. Structural and morphological characterization was performed using scanning electron microscopy (SEM), energy-dispersive spectroscopy (EDS), X-ray diffraction (XRD), and optical microscopy, confirming the successful incorporation of graphene. Electrochemical performance of the coating was evaluated through DC polarization and electrochemical impedance spectroscopy (EIS), it was found that the Ni-graphene composite coatings exhibited significantly enhanced corrosion resistance compared to pure Ni, with polarization resistance increasing from 90.165×10^3 Ω/cm² (pure Ni) to 168.133×10^3 Ω/cm² (Ni-Gr). Additionally, the inclusion of graphene nanosheets substantially improved microhardness, to 747.9 HV compared to pure Ni coatings (265 HV) which is attributed to dispersion strengthening and graphene's barrier properties. These results highlight graphene's potential as an effective reinforcement for nickel coatings, offering superior protection in saline and harsh environments, with promising applications across various industrial sectors.

O7. Atomic system: reticular spatial structure as engineering model of atomic shells and the meaning of the periodic table

Justyna Niewiadomska-Kaplar *
Tab edizioni, viale Manzoni, 24C - 00185 Roma (RM), Italy
+48 506265601, micromacro@ymail com

The structure of atoms has been described in this research work by introducing some innovative elementary theoretical concepts such as:

- interpretation of the electron pair not as a concentration of the electron cloud on one side of the nucleus, but as a symmetrical distribution of the electron cloud on both sides,

- hypothesis that in chemical bonds, one electron is shared, not an electron pair,

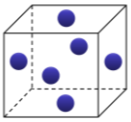
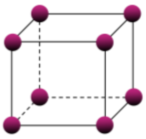
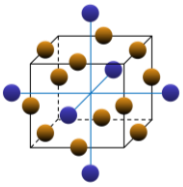
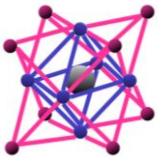
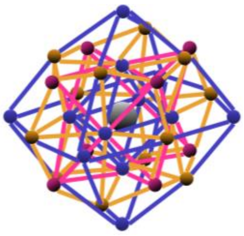
- interpretation of the transformation of the geometry of molecules in relation to the number of bonds as a result of changes in the spatial relationships between atoms, and not as a result of the hybridization of orbitals and prediction and calculation of the spatial parameters of molecules (topology, bond lengths and angles) by applying trigonometric equations and other geometric rules,

- hypothesis that electrons form atomic shells according to the technique of the multilayer spatial reticular structure, in which the lattice structure develops around a center and where the dynamics between electrons and nucleus and between electrons themselves play precise structural roles [1] [2]:

- the role of nodes of the reticular structure is carries out by localized electrons,
- the role of rods of the reticular structure is carries out by the mutual repulsion of electrons, both inside a shell and between electrons belonging to adjacent layers, which maintains an identical distance between them and makes this distance unalterable within the limits of thermodynamic equilibrium,
- the nodes of the atomic reticular structure are constrained by the central nucleus through the centripetal force of attraction of the nucleus towards the electrons.

The electrons of the atomic shells become localized precisely because they are stopped at a certain distance from the center by means of the mutual repulsion and attraction of the nucleus. The mutual repulsion of a group of localized electrons counteracts the force of attraction of the nucleus and prevents the structure from collapsing.

With this method the localized electrons form atomic shells in the shape of the following polyhedra:

octahedron **6** electrons $2p^6$ 	cube **8** electrons $3s^2$+$3p^6$ 	cuboctahedron + octahedron **18** electrons $4s^2$+$3d^{10}$+$4p^6$ 
Neon 	Argon 	Krypton 

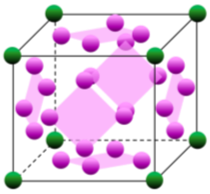
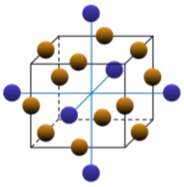
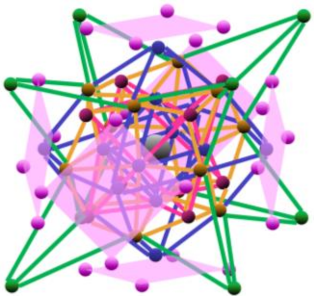
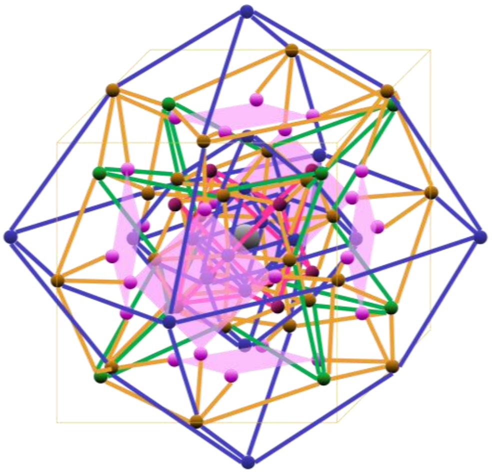
truncated octahedron + cube **32** electrons $5s^2$+$4d^{10}$ +$4f^{14}$+$5p^6$ 	cuboctahedron + octahedron **18** electrons $6s^2$+$5d^{10}$+$6p^6$ 
Ytterbium II inner shell 	Radon 

Fig. 1. Polyhedra formed by the localized electrons of atomic shells.

The subsequent shells are built by forming simple or composite tetrahedra between two layers of electrons. The tetrahedron is therefore the structural module of atomic shells.

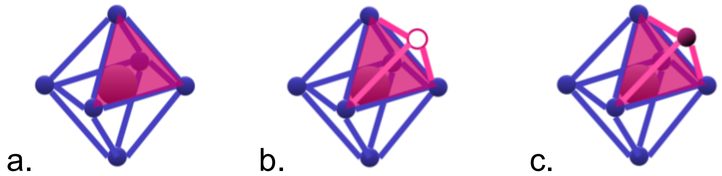


Fig. 2. a. Three electrons from the octahedral shell form the regular trigonal base of the tetrahedron which is completed by an electron from the new shell; b. An active site. c. The tetrahedron formed by the new electron and the three electrons from the previous shell.

Atomic space reticular structures have the ability to adapt their structure to changes in temperature/pressure. To illustrate this mechanism, magnesium hydrated salts will be analyzed. [3]

The atomic shells of many elements can exist with different structural options which determine different oxidation states. It will be investigated how two oxidation states of the p elements are determined by two structural options of the elements of the twelfth column of the periodic table: Zn, Cd and Hg.

References

[1] https://ettoreventrella.com/download/strutture-retcolari-spaziali/

[2] P. Casini, M. Vasta, *Scienza delle costruzioni*, Città Studi Edizioni, 2016.

[3] E. Hennings, H. Schmidt, W. Voigt, *"Crystal Structures of Hydrates of Simple Inorganic Salts. I. Water-Rich Magnesium Halide Hydrates* $MgCl_2\cdot 8H_2O$, $MgCl_2\cdot 12H_2O$, $MgBr_2\cdot 6H_2O$, $MgBr_2\cdot 9H_2O$, $MgI_2\cdot 8H_2O$ *and* $MgI_2\cdot 9H_2O$*",* Acta Crystallographica Section C Crystal Structure Communications, 2013.

O8. Therapeutic Assessment of Antidiabetic Efficiency of Co_3O_4 and TiO_2 Nanoparticles on alloxan-induced diabetic mice: An Experimental Study

Sammia Shahid [1] *

Department of Chemistry, School of Science, University of Management and Technology Lahore-54770 Pakistan
**Corresponding author: sammia.shahid@umt.edu.pk, 00923008864139*

Impaired glucose regulation and related consequences are hallmarks of diabetes mellitus, a global health concern. This study examines the potential of hydrothermally synthesized cobalt oxide and titanium dioxide nanoparticles in reducing diabetes in mice with alloxan-induced diabetes. Various characterization techniques were employed to confirm the successful fabrication of synthesized material, such as Energy-dispersive X-ray analysis for the determination of elemental composition UV-visible analysis, scanning electron microscopy (SEM) analysis for morphological investigation, and X-ray diffraction (XRD) studies for the crystal structure. By using quantitative real-time PCR to analyze the expression of liver-specific genes such as Glucokinase, Protein Kinase B, and immune response genes, their anti-diabetic efficacy was evaluated. However, to evaluate tissue integrity and therapeutic outcomes, histological analyses of the liver and spleen tissues were conducted. According to the study, when TiO_2 and Co_3O_4 NPs were used in conjunction with the common medication Glucophage, the expression of the GK, AKT, and IR genes was markedly increased, which led to improved cell uptake of glucose. These results imply that TiO_2 and Co_3O_4 NPs have hypoglycemic qualities and have the potential as affordable diabetic treatment agents. To prove them as practical therapeutic solutions for the treatment of diabetes, more investigation is necessary to assess their long-term safety, biocompatibility, and effectiveness. Histological examinations confirmed less inflammation and tissue damage. According to these results, TiO_2 and Co_3O_4 NPs have hypoglycemic and protective qualities, which makes them effective candidates for managing diabetes at a reasonable cost. To address any toxicological issues, long-term biocompatibility, and scalability for therapeutic applications, more research is necessary.

O9. Effect of different steel wires diameter on the reinforcement of jute/polyester resin composite

Bilal FETTAH [*]

LRM, Mechanical Engineering Department, Faculty of Technology, Hassiba Benbouali University of Chlef, P.O. Box 151, Esalem City, Chlef, 02000, Algeria

[*] *+2130672177661, ba.fettah@univ-chlef.dz*

Natural fibers such as jute are playing a crucial role across various industrial sectors. Jute fiber-reinforced composites are contributing to the development of eco-friendly applications. Innovative way to use jute with steel wires of small diameter in the reinforcement of the composite specimens with polyester resin for using in automotive, aerospace, marine and other civil infrastructure and structural application. The aim of this experimental work is to describe a novel fabrication of jute fiber reinforced steel metal wires of Ø=0.56mm, Ø=1mm, Ø=2.5mm respectively, investigation of properties and performance enhancements when four-layer jute and two-layer jute/two-layer glass composites are reinforced with these steel wires at different angle orientation 0°,45°and 90° (Fig.1). The incorporation of steel wires within the composites aims to leverage the high tensile strength of steel while maintaining the lightweight nature of jute fibers.

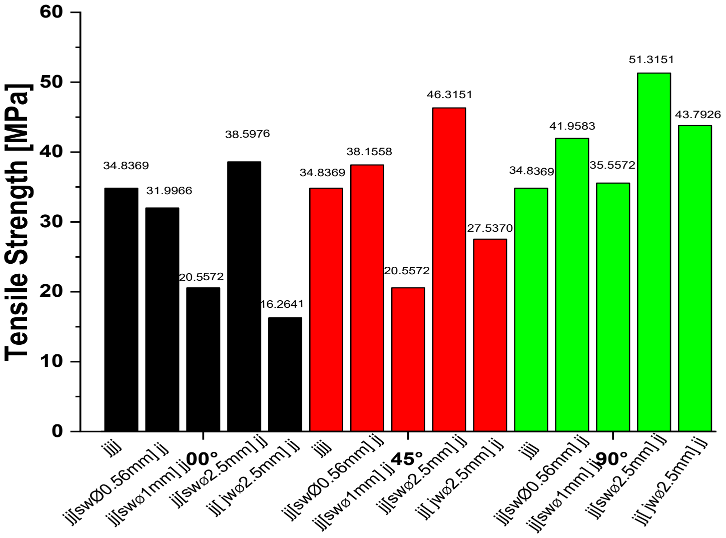


Fig. 1. Tensile strength for four-layer jute and two-layer jute/two-layer glass composites at different angle orientation 0°,45°and 90°.

O10. Development of Advanced Co-axial Phase Change Fibres for Thermoregulation of Civil Engineering Materials

Nathalia Hammes[1,2,*], José Monteiro[3], Elina Margarida Marinho[2],
Helena P. Felgueiras[2], M. Manuela P. Silva[4], Manuel F. M. Costa[5],
Iran Rocha Segundo[1,*],Joaquim Carneiro[1,*]

[1]*Centre of Physics of Minho and Porto Universities (CF-UM-UP), Campus Azurém, University of Minho, Av. da Universidade, 4800-058 Guimarães, Portugal*
[2]*Centre for Textile Science and Technology (2C2T-UMinho), Campus Azurém, University of Minho, Av. da Universidade, 4800-058 Guimarães, Portugal*
[3]*Earth Sciences Department of the University of Minho, Gualtar Campus, University of Minho, R. da Universidade, 4710-057 Braga, Portugal*
[4]*Centre of Chemistry of University of Minho (CQ-UMinho), Gualtar Campus, University of Minho, R. da Universidade, 4710-057 Braga, Portugal*
[5]*Centre of Physics of Minho and Porto Universities (CF-UM-UP), Gualtar Campus, University of Minho, R. da Universidade, 4710-057 Braga, Portugal*
[*]*E-mail: id11659@alunos.uminho.pt; iran@fisica.uminho.pt; carneiro@fisica.uminho.pt*

Rapid urbanisation and predominance of heat-retaining surfaces intensify the formation of Urban Heat Islands (UHIs), posing significant challenges to thermal comfort and urban sustainability. An innovative approach to mitigating urban heat islands (UHIs) involves incorporating phase change materials (PCMs) into civil engineering materials, leveraging thermoregulation through the latent heat principle. However, PCM leakage during phase transitions represents a significant challenge for their practical application. This study aims to develop and characterise co-axial polymeric phase change fibres (PCFs) with improved materials composition. PCFs were fabricated using polymeric materials, commercial cellulose acetate (CA) formed the protective sheath, and polyethylene glycol (PEG) served as the core. They were subsequently evaluated for their morphological, chemical, and thermal properties. The PCFs were efficiently developed to encapsulate the PCM into a core-shell structure, demonstrating effective thermal resistance and heat storage/release capabilities. The findings suggest that this technology holds substantial potential for applications in civil engineering materials, offering a sustainable approach to mitigate public health problems, reducing energy consumption with heating/cooling systems, and minimising environmental impacts.

O11. Effectiveness of TiO_2/MoS_2 nanocomposite electrodes prepared on ITO in the oxygen evolution reaction

Soner ÇAKAR[1,2,*], Mahmut ÖZACAR[2,3]

[1] *Zonguldak Bülent Ecevit University, Faculty of Science, Department of Chemistry, 67100 Zonguldak, Turkiye.*
[2] *Sakarya University, Biomaterials, Energy, Photocatalysis, Enzyme Technology, Nano & Advanced Materials, Additive Manufacturing, Environmental Applications and Sustainability Research & Development Group (BIOENAMS R&D Group), 54050 Sakarya, Turkiye.*
[3] *Sakarya University, Faculty of Science, Department of Chemistry, 54050 Sakarya, Turkiye.*
**Corresponding Author Tel.: +90 372 291 15 94. Fax: +90 372 257 41 81. cakarsoner@gmail.com*

- Abstract

In this work, TiO_2 and MoS_2 nanostructures were synthesized by hydrothermal methods. The synthesized nanocomposites were characterized by XRD and SEM techniques. A binary ITO/TiO2/MoS_2 nanocomposite was prepared by spin coating procedure and investigated its effects on photoelectrochemical water splitting. The ITO coated nanocomposites were analyzed by I-V curves under 150W halogen lamp.

- Introduction

The accelerating growth of the global population is driving an ever-increasing demand for energy. In the face of this mounting need, the depletion of fossil fuels has intensified scientific interest in the development of new and sustainable energy sources [1]. Among these, hydrogen energy is emerging as a technology with significant potential for the future. However, due to the cost and difficulties associated with storing hydrogen, studies on different techniques have gained momentum. Among these techniques, the production of H_2 and O_2 from water by photoelectrochemical method represents an environmentally friendly and innovative approach [2].

- Method

Synthesis and characterization of TiO_2 nanostructures

5 mL titanium isopropoxide (TIPP) and 1M NaOH were dissolved in 60 mL ultrapure water. The prepared white product was mixed in a magnetic stirrer for 1 h. The prepared solution was transferred to Teflon lined autoclave hydrothermal vessel. The hydrothermal vessel was heated at 150 °C for 12h. The synthesized TiO_2 structures were washed with pure water three times and ethanol twice and dried at 80°C overnight. The synthesized TiO_2 was characterized by XRD and SEM techniques.

Synthesis and characterization of MoS_2 nanostructures

5 mmol $(NH_4)_6Mo_7O_{24}\cdot 4H_2O$ (ammonium heptamolybdate tetrahydrate) and 10 mmol CH_4N_2S (thiourea) were dissolved in 50 mL ultrapure water. The pH of the solution was kept in the acidic region for good sulphurisation. The solution was mixed in a magnetic stirrer for 1 h and transferred Teflon lined autoclave vessel. The hydrothermal vessel was heated at 180 °C for 24h. The synthesized MoS_2 structures were washed with pure water

three times and ethanol twice and dried at 80°C overnight. The synthesized MoS$_2$ was characterized by XRD and SEM techniques.

Photoelectrochemical O$_2$ evaluation

The photoelectrochemical water dissociation reaction was examined by linear scanning voltammetry technique in 1 M H2SO$_4$ environment using a conventional electrochemical cell prepared with TiO$_2$/MoS$_2$ nanostructures working electrode coated on ITO glass, Pt wire counter electrode and Ag/AgCl reference electrode. At the photoelectrochemical examination of the decomposition of water, a 100W halogen lamp stimulated the solution and the working electrode during the measurement. In addition, both H$_2$ production efficiency and O$_2$ production efficiency were investigated by taking electrochemical impedance curves and Tafel curves for the purpose of studying conductivity behavior.

- Results

The XRD results of the synthesized nanomaterials are presented in Figure 1. The XRD spectra indicate that the TiO$_2$ nanoparticles are indexed in the anatase crystal structure. The unit cell parameters a, c, V and the space group of TiO$_2$ anatase form are 3.515 Å, 9.26 Å, 135.42 Å^3, Fm3m, respectively. MoS$_2$ nanoparticles have hexagonal unit cell and unit cell parameters a, c, V and space group are 3.145 Å, 12.51 Å, 107.12 Å^3, P63/mmc, respectively. Furthermore, the crystal sizes calculated by the Debye–Scherrer equation are 31.2 nm and 41.3 nm for TiO$_2$ and MoS$_2$, respectively.

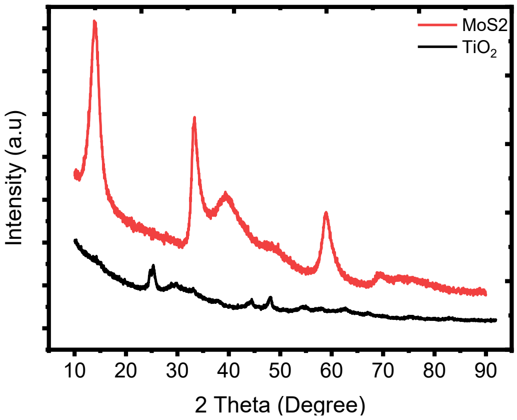


Fig. 1. The XRD patterns of synthesized nanostructures.

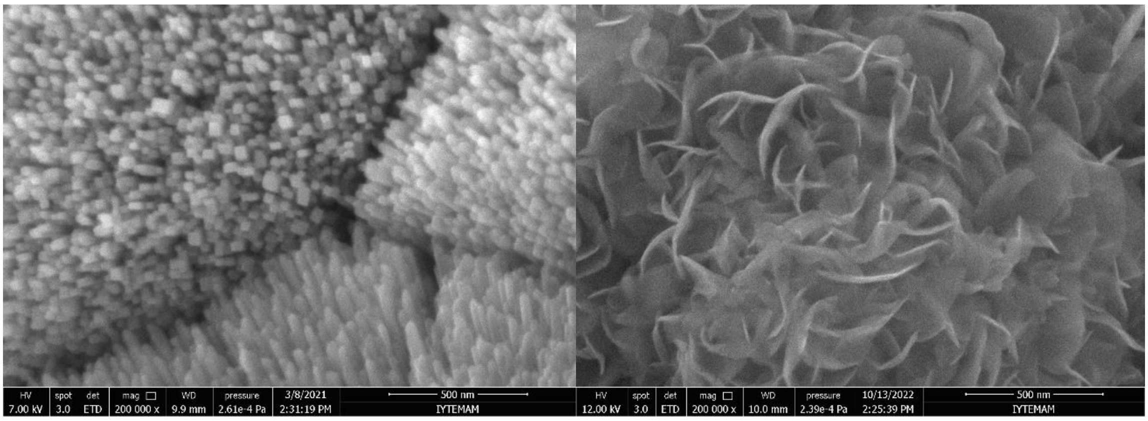


Fig 2. FE-SEM images of TiO$_2$ (A) and MoS$_2$ (B).

- Discussion

The present study concerns the photoelectrochemical OER applications of TiO_2 and MoS_2 composite electrodes. In this study, TiO_2 and MoS_2 nanoparticles were synthesized by the hydrothermal method and coated on ITO glass by the spin coating method. The oxygen effect produced photoelectrochemically was analyzed by means of I-V and Tafel curves in OER measurements. It was observed that the oxygen evolution reaction (OER) efficiency of the prepared composite electrodes increased by 10% compared to pristine TiO_2 and MoS_2. It is observed to have photo induced charge carriers and stagnant water oxidation kinetics. In order to cincrease the photocurrent intensity of these oxide photoanodes in visible light, a new approach can be developed by developing hybridization with noble metal nanoparticles to increase efficiency.

References

[1] F. Khodabandeh, H. Abdizadeh, A.A., Avanaki, M.R., Golobostanfard, *International Journal of Hydrogen Energy*, **65**, 779-803, 2024.

[2] E., Marchini, S., Caramori, S., Carli, Molecules, **29**, 293, 2024.

O12. Acacia gum-graft Copolymer Hydrogel: Preparation and Metal ions Adsorption studies

Sirajo Abubakar Zauro[1*] , Abdullahi Ibrahim Tsafe[2], Shamsuddeen Yahaya[1]

[1] Department of Energy and Applied Chemistry, Usmanu Danfodiyo University, Sokoto, PMB 2346, Sokoto, Nigeria
[2] Department of Pure and Environmental Chemistry, Usmanu Danfodiyo University, Sokoto, PMB 2346, Sokoto, Nigeria

[*]Telephone number: +234703563131, Email: sirajo.abubakar@udusok.edu.ng

The graft copolymer hydrogel (Acacia gum-graft-poly [(N, N-dimethylacrylamide)-co-(2-acrylamido-2-methylpropanesulfonic acid)] was synthesized using N,N-bisacrylamide (MBA) as cross linker and potassium per sulphate (KPS) as initiator via microwave irradiation technique. The graft copolymer hydrogel was characterized using Fourier transform infrared (FTIR), thermogravimetric analysis (TGA) and X-ray spectroscopy (EDS) techniques. The effects of contact time, adsorbent dose, metal ions initial concentration of the adsorbate solution on the adsorption capacity of the graft copolymer hydrogel was evaluated. Kinetics and isotherms parameters of adsorption were also evaluated. The kinetic study indicated that the adsorption of both $Pb^{2+}$and Cd^{2+}ions follow pseudo second order kinetic model. The adsorption isotherms for both $Pb^{2+}$and Cd^{2+}ions correlate well with the Freundlich model. The highest adsorption capacity of 167.5 mg/g and 188 mg/g for $Pb^{2+}$and Cd^{2+} respectively were recorded after 300 minutes.

O13. $TiO_2/SiO_2/MAPbCl_3$ photocatalyst for tartrazine removal: Synthesis, characterization and reusability

Oumayma BOUHAJEB[1,2 *], Ramzi HAMMAMI[1], Mahmut ÖZACAR[2,3], Adel MEGRICHE[1]

[1] Laboratoire de Chimie Minérale Appliquée (LCMA) LR19ES02, Faculté des Sciences de Tunis, Université Tunis El Manar. Campus Universitaire Farhat HACHED, 2092, El Manar –Tunis, Tunisie
[2] Sakarya University, Biomaterials, Energy, Photocatalysis, Enzyme Technology, Nano & Advanced Materials, Additive Manufacturing, Environmental Applications and Sustainability Research & Development Group (BIOENAMS R&D Group), 54050 Sakarya, Turkiye.
[3] Sakarya University, Faculty of Science, Department of Chemistry, 54050 Sakarya, Turkiye.
[*] Corresponding Author Tel.: +21624499567, e-mail address: oumayma.bouhajeb@etudiant-fst.utm.tn

-Abstract: In this work $TiO_2/SiO_2/MAPbCl_3$ photocatalysts with different $MAPbCl_3$ content (TiO_2/SiO_2 composite' 25%, 50%, and 75%), were synthesized via ultrasound-assisted colloidal method and characterized through various technics. Structural features were verified via FTIR and XRD, while optical analysis revealed that the $TiO_2/SiO_2/MAPbCl_3$ composite with 75% $MAPbCl_3$ exhibited superior visible-light absorption and the lowest band gap value (E_g = 3.01 eV). The photocatalytic performance of synthesized composites was appraised for the degradation of Tartrazine at visible light for over 180 minutes. Among the tested materials, $TiO_2/SiO_2/MAPbCl_3$(75) achieved also the highest degradation efficiency of 84.93%. The reusability test indicated a performance decline of approximately 9% over three cycles.

-Introduction: While $MAPbCl_3$ has been commonly utilized in numerous applications because of its low price and excellent optoelectronic properties [1], SiO_2, with its high surface area, is often employed as a support material to enhance the stability and dispersion of active photocatalysts. Combining these materials with TiO_2 [2], a well-known photocatalyst, can lead to improved photocatalytic performance, particularly in the visible-light range. However, optimizing the composition and understanding the synergistic effects of these components remain critical for achieving high efficiency in environmental applications.

-Method:

TiO_2/SiO_2 composite synthesis: TiO_2 suspension was prepared in ethanol (80 mL) and sonicated for 30 minutes. After adding SiO_2 to the TiO_2 dispersion at a mass ratio of 85:15, sonication continued for another 30 minutes and then mixed at 70°C until a colloidal appearance was formed. The solid separated from the mixture was dried at 100°C for 2 hours and then subjected to heat treatment at 500°C for 2 hours. The final product was ground to obtain TiO_2/SiO_2 nanocomposite.

$TiO_2/SiO_2/MAPbCl_3$ composite synthesis: After dispersing 0.4 g of TiO_2/SiO_2 nanocomposite in 20/20 mL volume ratio ethanol/water mixture, previously synthesized $MAPbCl_3$ perovskite was supplemented at 25%, 50% and 75% ratios and sonicated for 30 min. The final products were dried at 80°C overnight.

-Results:
XRD patterns confirm the successful synthesis of $TiO_2/SiO_2/MAPbCl_3$ nanocomposites, with characteristic peaks of $MAPbCl_3$ and TiO_2 present, while SiO_2 remains amorphous.

The results indicate preserved crystallinity and effective integration of $MAPbCl_3$ into the composite structure.

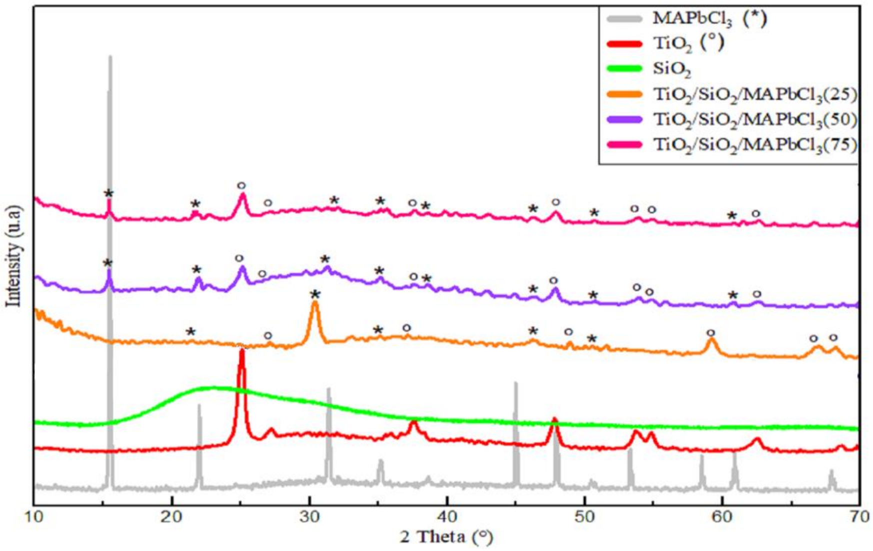


Fig. 1. XRD patterns of simple and composite materials [3]

UV-Vis DRS results (Fig. 2(a)) show that increasing the $MAPbCl_3$ content enhances visible-light absorption. All samples have an absorption edge around 400 nm, confirming their potential for visible-light-driven applications. The improved absorption suggests that photocatalytic efficiency will be better for the higher $MAPbCl_3$ content composites.

The reduced PL intensity (Fig. 2(b)) in $TiO_2/SiO_2/MAPbCl_3$ composites, especially in the 75% $MAPbCl_3$ composite, suggests improved charge carrier dynamics, potentially leading to higher photocatalytic performance.

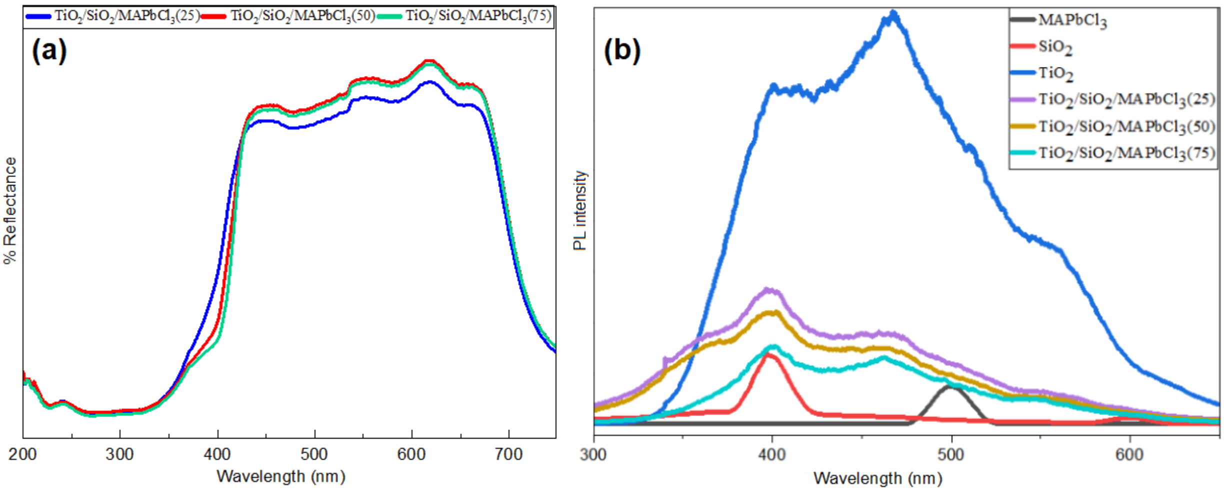


Fig. 2. UV-DRS (a) and PL (b) spectra of samples [3]

-Discussion:

The present study focuses on the photocatalytic degradation of Tartrazine via $TiO_2/SiO_2/MAPbCl_3$ composites with varying $MAPbCl_3$ content (25%, 50%, and 75%)

under visible-light irradiation. Photocatalysts were synthesized via ultrasound- colloidal process, characterized and investigated their photocatalytic efficiencies. The $TiO_2/SiO_2/MAPbCl_3$ composite with 75% $MAPbCl_3$ exhibited the highest visible-light absorption of 84.93% over 180 min and its reusability was evaluated over 3 cycles.

References

[1] S. Parwaiz, M.M. Khan, Perovskites and perovskite-based heterostructures for photocatalytic energy and environmental applications, J. Environ. Chem. Eng. 12 (2024) 113175.

[2] M.-W. Zheng, Y.-R. Lin, S.-H. Liu, TiO_2@g-C_3N_4/SiO_2 with superior visible-light degradation of formaldehyde for indoor humidity control coatings, Mater. Today Sustain. 24 (2023) 100496.

[3] O. Bouhajeb, R. Hammami, A. Megriche, M. Özacar, Improving TiO_2/SiO_2 activity with $[CH_3NH_3]PbCl_3$ addition for tartrazine photocatalytic degradation under UV and visible light irradiations, Inorg. Chem. Commun. 174 (2025) 113992.

O14. Mn doping $MAPbCl_3/TiO_2/SiO_2$: A promising strategy for less lead perovskite based photocatalyst toward tartrazine degradation

Oumayma BOUHAJEB[1,2 *], Ramzi HAMMAMI[1], Mahmut ÖZACAR[2,3,] Adel MEGRICHE[1]

[1] Laboratoire de Chimie Minérale Appliquée (LCMA) LR19ES02, Faculté des Sciences de Tunis, Université Tunis El Manar. Campus Universitaire Farhat HACHED, 2092, El Manar –Tunis, Tunisie

[2] Sakarya University, Biomaterials, Energy, Photocatalysis, Enzyme Technology, Nano & Advanced Materials, Additive Manufacturing, Environmental Applications and Sustainability Research & Development Group (BIOENAMS R&D Group), 54050 Sakarya, Turkiye.

[3] Sakarya University, Faculty of Science, Department of Chemistry, 54050 Sakarya, Turkiye.

[*] Corresponding Author Tel.: +21624499567, e-mail address: oumayma.bouhajeb@etudiant-fst.utm.tn

-Abstract: In this work, we explore the effect of Mn doping on $MAPbCl_3$ (MAPC) perovskite and its impact on the photocatalytic activity of TiO_2/SiO_2 heterostructure for the tartrazine degradation at visible light irradiation. Structural and optical characterizations confirm the successful incorporation of Mn^{2+} [1], leading to enhanced charge separation, increased light absorption in the visible spectrum, and improved photocatalytic efficiency [2]. Mn-doped $MAPbCl_3$ based heterostructure exhibited superior degradation efficiency 92.87% under visible light. Furthermore, stability tests confirmed the material's robustness, with minimal efficiency loss, paving the way for more effective wastewater treatment solutions.

-Introduction: This study explores a novel photocatalytic composite where Mn-doped $MAPbCl_3$ is integrated with a TiO_2/SiO_2 heterostructure to enhance dye degradation while reducing lead content. Mn doping improves visible-light absorption and charge separation, and the TiO_2/SiO_2 composite provides additional stability, making the composite a promising candidate for sustainable wastewater treatment.

-Method:

Photocatalysts synthesis: TiO_2 was dispersed in an ethanol solution and sonicated for 30 minutes, followed by the addition of SiO_2 and further sonication. The resulting mixture was heated at 70°C under stirring until it acquired a colloidal appearance, then dried at 100°C for 2 hours and calcined at 500°C for 2 hours. The calcined product was ground to obtain a homogeneous TiO_2/SiO_2 powder, which was then mixed in an ethanol-water solution with perovskite samples at a 3:1 ratio, sonicated for 30 minutes, and dried overnight at 80°C.

-Results:

XRD patterns of $MnCl_2$, undoped (MAPC) and Mn doped (Mn20, Mn40, Mn50, Mn60 and Mn80) shown in Fig.1 demonstrate a preserved cubic structure for all Mn doped perovskites whatever the concentration of Mn^{2+}, the purer phase was obtained for Mn80 where the dope percentage was about 80%. The first peak corresponding to (100) shift toward higher 2 theta when the Mn^{2+} concentration increases which can be attributed to the progressive lattice contraction.

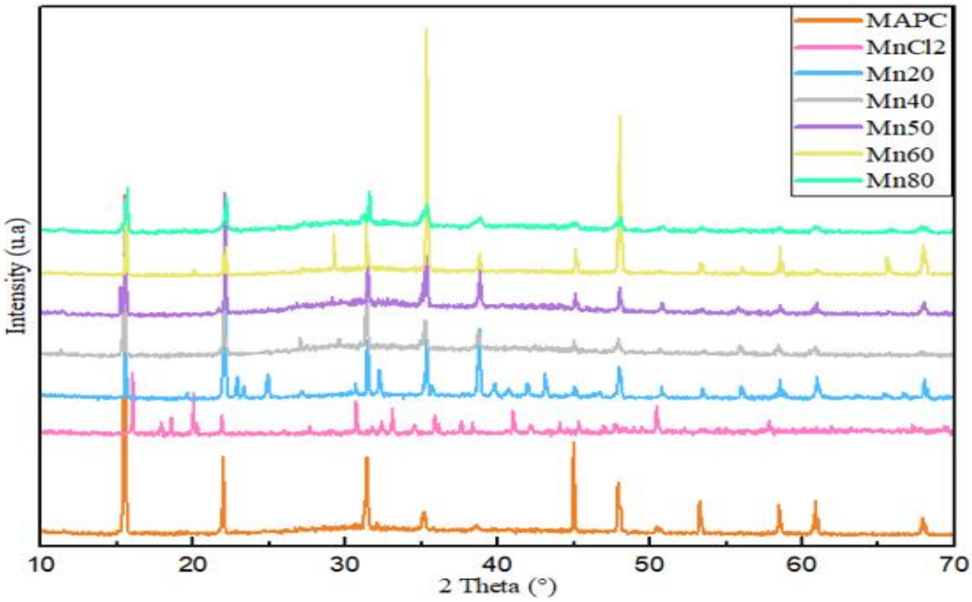


Fig.1. XRD patterns of synthesized doped and undoped perovskites and $MnCl_2$ precursor

Gap energy of undoped and Mn-doped $MAPbCl_3$ were determined using Kubelka-Munk function demonstrating a decrease for all-doped perovskites particularly for 80% Mn doped (Mn80) where E_g become 2.87 eV.

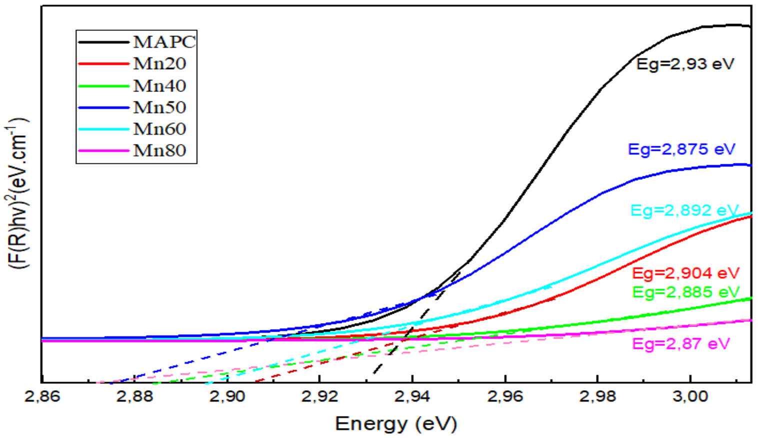
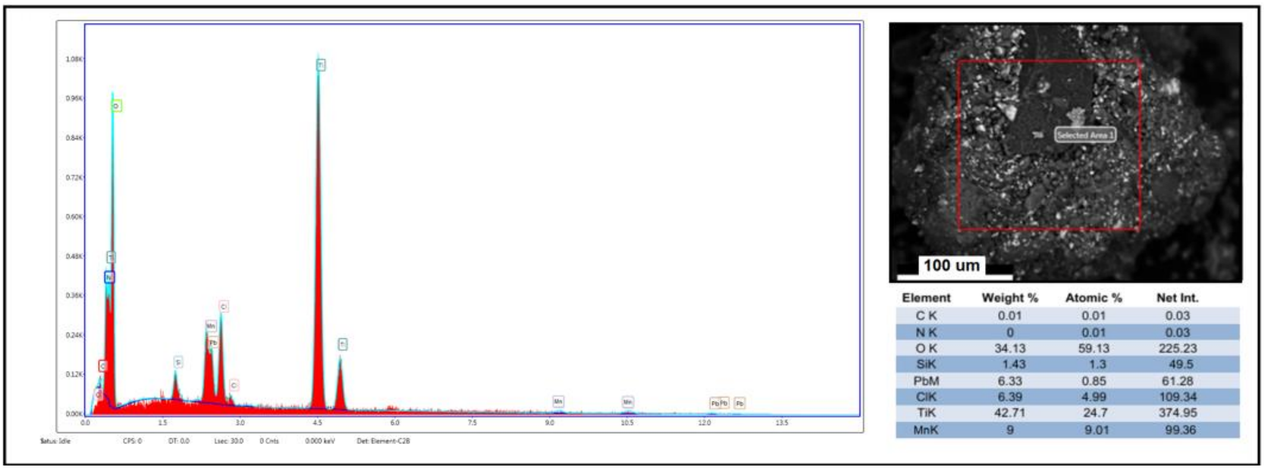


Fig. 2. Gap energy estimation of doped and undoped perovskites

The incorporation of Mn seems to reduce the lead content. EDX analysis (Fig.3) shows a decrease in lead content expected for pure $MAPbCl_3$. This may result from Mn (along with TiO_2 and SiO_2) substituting or diluting the Pb content.



Element	Weight %	Atomic %	Net Int.
C K	0.01	0.01	0.03
N K	0	0.01	0.03
O K	34.13	59.13	225.23
SiK	1.43	1.3	49.5
PbM	6.33	0.85	61.28
ClK	6.39	4.99	109.34
TiK	42.71	24.7	374.95
MnK	9	9.01	99.36

Fig. 3. EDX spectra of Mn:$MAPbCl_3/TiO_2/SiO_2$ and its elemental analysis

-Discussion:

Structural analysis confirmed that Mn doping preserves the cubic structure of $MAPbCl_3$ while causing lattice contraction and reducing the band gap, which boosts photocatalytic efficiency. TiO_2/SiO_2 support further decreases lead content and enhances material stability, resulting in effective tartrazine degradation under visible light.

References

[1] B.P. Kore, S. Das, D.D. Sarma, Temperature-dependent anomalous Mn^{2+} emission and excited state dynamics in Mn^{2+}-doped $MAPbCl_{3-x}Br_x$ nanocrystals, Journal of Chemical Sciences 133 (2021) 64.

[2] J. Kong, W. Zhang, Y. Zhang, M. Xia, X. Wu, Y. Wang, Enhancing Photocatalytic Activity on (MnO@TNTAs):Mn^{2+} with a Hierarchical Sandwich-Like Nanostructure via a Two-Step Procedure, J Electron Mater 47 (2018) 2800–2807.

O15. Innovative Multifunctional Hydrogel Dressings with Natural Antimicrobial Extracts for Enhanced Diabetic Wound Healing

Muhammet Kamil Kerim[1,2, *], Mahmut ÖZACAR[2,3]

[1] Sakarya University, Institute of Natural Sciences, Department of Biomedical Engineering, 54187, Sakarya, Turkiye.
[2] Sakarya University, Biomaterials, Energy, Photocatalysis, Enzyme Technology, Nano & Advanced Materials, Additive Manufacturing, Environmental Applications and Sustainability Research & Development Group (BIOENAMS R&D Group), 54050 Sakarya, Turkiye
[3] Sakarya University, Faculty of Science, Department of Chemistry, 54050 Sakarya, Turkiye
** Presenter's telephone, fax and e-mail address: +90 561 615 09 54, +90 264 295 59 50 and Mkamilkerim@gmail.com*

Abstract

Diabetic wound management remains a critical challenge due to prolonged healing times, high infection risks, and limited cost-effective solutions. This study proposes the development of multifunctional hydrogel dressings using biocompatible polymers (PVA and PVP) integrated with antimicrobial plant extract (*Salvadora persica*) to address these challenges. The hydrogels were synthesized through crosslinking and freeze-thaw methods, with structural characterization via SEM, FTIR, and mechanical testing to assess porosity, hydration capacity, and stability. Antibacterial efficacy was evaluated against common pathogens such as S. aureus and E. coli, while biocompatibility was tested using fibroblast cell cultures. Controlled release of bioactive compounds from plant extract was investigated to enhance therapeutic outcomes.

Introduction

Diabetic wounds pose a significant healthcare challenge due to chronic inflammation, impaired angiogenesis, formation of bacterial colonization and increase in the levels of reactive oxygen species. These complications delay the natural healing process, making diabetic wounds prone to infections and increasing the risk of severe complications, including lower limb amputations. Given the limitations of conventional wound dressings in addressing these complexities, advanced biomaterials such as hydrogels have gained attention for their ability to provide an optimal healing environment [1]. Hydrogels, particularly those based on polyvinyl alcohol (PVA) and polyvinylpyrrolidone (PVP), are widely recognized for their biocompatibility, biodegradability, and water solubility. PVA exhibits excellent chemical resistance but has low hydrophilicity, making it rigid in film formation. To overcome this limitation, blending PVA with PVP is recommended, as PVP enhances water compatibility and flexibility of the resulting films. This combination makes PVA/PVP hydrogels promising candidates for wound healing applications, particularly when integrated with bioactive compounds that can accelerate the repair process. Therefore, to enhance the therapeutic potential of PVA/PVP hydrogels, natural plant extracts with antimicrobial, anti-inflammatory, and antioxidant properties can be incorporated. Studies have demonstrated that plant-based bioactive compounds, such as phenolics and alkaloids, contribute to wound healing by modulating inflammation, promoting tissue regeneration, and protecting against oxidative damage [2,3]. This study aimed to develop a PVA/PVP hydrogel loaded with bioactive extract from *Salvadora persica* (antimicrobial). The structural, mechanical, and biological properties of the hydrogel were systematically evaluated to determine its suitability for diabetic wound management.

Method

Initially, 0.8 g of PVA was solved in 10 mL of deionized water (DW) at 90°C continuously stirring for 2 hours. Meanwhile, 0.8 g of PVP was dissolved in a separate 10 mL of DW at 50°C, also stirring, for 1 hour. Once both solutions achieved transparency, they were mixed in a 1:1 ratio at 50°C until a homogeneous blend was obtained. The resulting mixture was then divided into two portions for the two different incorporation methods of the antimicrobial plant extract:

Incorporation of plant extract during hydrogel synthesis: The plant extract was directly added into the PVA/PVP blend prior to the freeze-thaw process. After thorough mixing at 50°C to ensure uniform dispersion, the solution was poured into the Petri dish and left uncovered at ambient conditions overnight to eliminate air bubbles. The hydrogel was then subjected to four consecutive freeze-thaw cycles, each including freezing at −20°C for 24 hours and thawing at 4°C for 6 hours.

Post-loading of plant extract into preformed hydrogel: In parallel, a portion of the PVA/PVP mixture without the plant extract was cast into a Petri dish, degassed overnight, and subjected to the same four freeze-thaw cycles to form a blank hydrogel. After the final thaw, the preformed hydrogel was immersed in a solution containing the antimicrobial plant extract at room temperature. This post-loading step allowed diffusion of the extract into the porous hydrogel network.

For both approaches, the loading efficiency and subsequent release of the plant extract were monitored by UV-Vis spectroscopy. Finally, functional group analysis was conducted by FT-IR spectroscopy to confirm the successful incorporation of the polymers and the antimicrobial agent.

Results

The freeze-thaw cycles yielded stable PVA/PVP hydrogels with desirable mechanical integrity and a porous network suitable for loading bioactive molecules. FT-IR analysis verified the presence of characteristic peaks corresponding to both polymers and indicated successful integration of the antimicrobial plant extract in each method. UV-Vis data revealed that both the in-synthesis and post-loading strategies facilitated the release of the plant extract over time, with variations in release profiles and potential applications depending on the chosen loading method. These findings suggest that the PVA/PVP hydrogel system is a promising platform for delivering antimicrobial agents, offering versatile options for incorporation and sustained release in wound care or related biomedical applications.

Discussion

The stable PVA/PVP hydrogel network, formed via freeze-thaw cycles, effectively supported both in-synthesis and post-loading of an antimicrobial plant extract. The in-synthesis approach yielded a uniform distribution and faster initial release, whereas post-loading provided a more prolonged release profile. Thus, these hydrogels are promising for versatile wound care applications requiring sustained antimicrobial efficacy.

References

[1] J.L. Burgess, W. A. Wyant, B. Abdo Abujamra, R.S. Kirsner, and I. Jozic, Medicina, 57(10), 1072 (2021).

[2] S.A. Soud, B.A. Hasoon, A.I. Abdulwahab, N.N. Hussein, and R.K. Maeh, EurAsian Journal of BioSciences, 14(2), 2921-2931 (2020).

[3] M. Veiga, E.M. Costa, S. Silva, and M. Pintado, Critical reviews in food science and nutrition, 60(5), 873-886 (2020).

O16. Synthesis, swelling behavior and water retention capacity of self-healing gelatin-chitosan-silk sericin hydrogels

Selen Şakar[1,2,*], Mahmut ÖZACAR[2,3]

[1] Sakarya University, Institute of Natural Sciences, Department of Chemistry, 54187, Sakarya, Turkiye
[2] Sakarya University, Biomaterials, Energy, Photocatalysis, Enzyme Technology, Nano & Advanced Materials, Additive Manufacturing, Environmental Applications and Sustainability Research & Development Group (BIOENAMS R&D Group), 54050 Sakarya, Turkiye
[3] Sakarya University, Faculty of Science, Department of Chemistry, 54050 Sakarya, Turkiye
* Presenter's telephone, fax and e-mail address: +90 264 295 67 86, +90 264 295 59 50 and selen.sakar@ogr.sakarya.edu.tr

Abstract

In this study, hybrid hydrogels containing chitosan (CS), gelatin (GEL), and varying amounts of silk sericin (SS) were investigated. The effect of adding different amounts of SS on the water retention capacity and swelling behavior of the hydrogel was perused, and the self-healing features of the hydrogels were observed using an optical microscope. As a result, the hydrogels demonstrated self-healing features without any external stimulus, exhibiting similar water retention capacity and high swelling behavior.

Introduction

Self-healing hydrogels, developed through various cross-linking methods, are three-dimensional polymeric networks that can mimic biological tissue when swollen by absorbing large amounts of water. They can repair themselves when damaged without any external stimulus. These hydrogels are composed via the chemical or physical crosslinking of natural, synthetic, or hybrid polymer materials. Physically crosslinked hydrogels have weak mechanical strength, and environmental conditions may lead to the degradation of the polymer networks. For this reason, the use of chemical crosslinkers is common [1, 2]. The production of hydrogels to be used in biomedical applications from natural polymers provides advantages in terms of non-toxicity, biocompatibility and biodegradability [3]. Chitosan is a naturally abundant polymer, second only to cellulose, and is widely used because of its features like biocompatibility, non-toxicity, and biodegradability [3, 4]. Gelatin has features like non-toxicity, biodegradability, and biocompatibility, and can absorb water up to 5-10 fold its weight [3, 5]. Sericin, a natural protein, possesses features like biodegradable, antioxidant, anticancer, and biocompatibility. However, it is recommended to blend it with other polymers to improve its weak mechanical features [6, 7]. The aim of this study is to synthesize self-healing CS-GEL-SS hydrogels and investigate their swelling behavior and water retention capacity.

Method

In the study, silk sericin was first obtained from silkworm cocoons. To do this, the silkworm cocoons were cut into small pieces, and 50 mL of deionized water (DW) was added to 5 g of cocoon, which was then placed in a hydrothermal autoclave reactor. The suspension was autoclaved for 30 min at 120°C, after which the cocoon proteins, sericin and fibroin, were separated by filtration using filter paper. The resulting sericin solution was left in the freezer for 24 hours, and then lyophilized to obtain sericin powder. To obtain the 2.6%

(w/v) sericin solution, powdered silk sericin was dissolved in DW at 85°C for 2 h using a magnetic stirrer. To acquired 2% (w/v) chitosan solution, chitosan was dissolved in a 2% (v/v) acetic acid solution at ambient conditions for 2 h mixing a magnetic stirrer. To prepare 10% (w/v) gelatin solution, gelatin was dissolved in DW at 50°C for 1 h using a magnetic stirrer. The prepared polymer solutions were mixed in specific volume ratios until homogeneous, and 4% of the total volume of glycerol was supplemented as a plasticizer. The mixture was stirred for 20 minutes using a magnetic stirrer. Finally, citric acid, a natural crosslinking agent, was added at 20% of the total polymer weight, and the entire mixture was stirred for 24 h at 40°C. The resulting solutions were transferred into Petri dishes for hydrogel formation, and gelation was allowed to occur for 48 h. The formed hydrogels were subjected to freeze-thaw cycles for 5 cycles, after which their self-healing properties were observed using an optical microscope, and swelling and water retention tests were applied to the hydrogels.

Results

After the initial images of the hydrogels were taken under an optical microscope, scratches were made on them using a razor blade, and the images were taken again. After 5 and 15 minutes, the images were captured again, and the self-healing properties were confirmed. The lyophilized hydrogels were put in 15 mL Falcon tubes and 10 mL of DW was supplemented before the swelling test. The swelling analysis continued until the hydrogels' water capacity reached equilibrium. It was determined that the synthesized hydrogels had a high swelling capacity. To determine the water retention capacity, the mass of the hydrogels was weighed before and after being kept in DW at ambient conditions for 24 h. The hydrogels were then left to dry in an oven at 37°C, and measurements were taken at specific time periods. The water retention capacity of the prepared hydrogels showed similar results.

Discussion

The synthesized CS-GEL-SS hydrogels were observed to self-heal using an optical microscope. It was determined that the hydrogels had a high swelling capacity and exhibited similar water retention capacity.

References

[1] M. Ginting, S.P. Pasaribu, I. Masmur, J. Kaban, and Hestina, *RSC Advances*, **10(9),** 5050–5057 (2020).

[2] K. Mali, S. Dhawale, R. Dias, N. Dhane, and V. Ghorpade, *Indian Journal of Pharmaceutical Sciences*, **80**, 657–667 (2018).

[3] S. Patel, S. Srivastava, M.R. Singh, and D. Singh, *International Journal of Biological Macromolecules*, **107**, 1888–1897 (2018).

[4] J. Saha, M.I.H. Mondal, F. Ahmed, and M. Rahman, *Arabian Journal of Chemistry*, **16(9)**, 105087 (2023).

[5] L. Fan, H. Yang, J. Yang, M. Peng, and J. Hu, *Carbohydrate Polymers*, **146**, 427–434 (2016).

[6] B.M. Bakadia, L. Lamboni, A.A.Q. Ahmed, R. Zheng, B.O.O. Boni, Z. Shi, S. Song, T. Souho, B.M. Mukole, F. Qi, and G. Yang, *Smart Materials in Medicine*, **4**, 37–58 (2023).

[7] G. Tao, Y. Wang, R. Cai, H. Chang, K. Song, H. Zuo, P. Zhao, Q. Xia, and H. He, *Materials Science and Engineering: C*, **101**, 341–351 (2019).

O17. Synthesis, Characterization, and Drug Release Profile of PEG-Coated Fe_3O_4 Magnetic Nanoparticles Loaded with Dexamethasone

Mahsa Heidarnejad[1,2*], Münteha Özsoy[2,3], Mahmut Özacar[2,4]

[1]Sakarya University, Institute of Natural Sciences, Department of Chemistry, 54187 Sakarya, Turkiye
[2]Sakarya University, Biomaterials, Energy, Photocatalysis, Enzyme Technology, Nano & Advanced Materials, Additive Manufacturing, Environmental Applications and Sustainability Research & Development Group (BIOENAMS R&D Group), 54050 Sakarya, Turkiye
[3]Department of Pharmaceutical Toxicology, Faculty of Pharmacy, Kocaeli Healthy and Technology University, Başiskele 41190, Kocaeli, Turkey
[4]Sakarya University, Faculty of Science, Department of Chemistry, 54050 Sakarya, Turkiye
. Presenter's telephone, fax and e-mail address: +90 264 295 67 86, +90 264 295 59 50 and Heidarnejadmahsa@gmail.com*

Abstract

In recent years, magnetic nanoparticles (MNPs) have received considerable interest in drug delivery applications because of their biocompatibility, high surface area, and magnetic properties. In this study, Fe_3O_4 MNPs were synthesized and coated with polyethylene glycol (PEG) to improve their stability and biocompatibility for dexamethasone delivery. Dexamethasone, a widely used anti-inflammatory drug, was loaded onto PEG-functionalized Fe_3O_4 MNPs, and its loading efficiency and release behavior were evaluated. The MNPs were via Scanning Electron Microscopy (SEM), Fourier Transform Infrared (FTIR) and Ultraviolet-Visible (UV-VIS) Spectroscopies to confirm structural modifications and drug interaction. Drug release studies were conducted under physiological conditions to analyze the controlled release profile. The results demonstrated efficient dexamethasone loading, stable nanoparticle morphology, and sustained drug release, suggesting that PEG-coated Fe_3O_4 MNPs have potential as an effective drug carrier system.

Introduction

Magnetic nanoparticles (MNPs), particularly Fe_3O_4, have been widely explored for biomedical implementations because of their superparamagnetic features, easy surface modification, and biocompatibility [1]. The ability to functionalize Fe_3O_4 MNPs with polymeric coatings, such as polyethylene glycol (PEG), enhances their dispersion, reduces aggregation, and prolongs circulation time in biological systems [2]. PEGylation also prevents rapid clearance by the immune system, making it a suitable approach for drug delivery applications.

Dexamethasone, a potent glucocorticoid with anti-inflammatory and immunosuppressive properties, is commonly used for treating various inflammatory diseases [3]. However, systemic administration often leads to adverse effects such as osteoporosis, hyperglycemia, and immune suppression [4]. Therefore, designing a controlled-release drug delivery system can minimize these side effects while enhancing therapeutic efficiency. In this study, PEG-coated Fe_3O_4 MNPs were synthesized, and their potential as a dexamethasone carrier was evaluated through characterization and drug release studies under physiological conditions.

Method

The MNPs were synthesized using a co-precipitation method. In a nitrogen-filled environment, 3.65g (0.0135 mol) of $FeCl_3·6H_2O$ and 2.1 g (0.0123 mol) of $FeSO_4·H_2O$ were dissolved in distilled water (DW). The solution was heated to 80 °C and mixed at 150 rpm for 1 h. Subsequently, ammonia solution (22.5 mL) was quickly supplemented to the solution and stirred for another hour under nitrogen atmosphere. The resulting MNPs were then cooled to room temperature. Afterward, the MNPs were washed several times with DW and once with ethanol. Finally, they were dried for 24 h at 65 °C to obtain the desired product. The synthesized MNPs were characterized using various techniques such as XRD, SEM and FTIR. The loading and releasing of salicylic acid were evaluated using UV-Vis spectroscopy [5].

Results

To verify the successfully synthesis and functionalization of PEG-coated Fe_3O_4 MNPs loaded with dexamethasone, various characterization techniques were employed: Scanning Electron Microscopy (SEM), analysis was performed to specify the microstructure, particle size, and surface structure of the [6]. Fourier Transform Infrared Spectroscopy (FTIR), spectra were employed to identify characteristic functional groups of Fe_3O_4, PEG, and dexamethasone, confirming successful surface modification and drug loading [1]. Ultraviolet-Visible Spectroscopy (UV-VIS), analysis was used to monitor dexamethasone loading efficiency by detecting its characteristic absorption peaks before and after nanoparticle loading [2]. Drug Loading and Release Studies: The amount of dexamethasone loaded onto PEG-coated Fe_3O_4 MNPs was quantified, and drug release studies were conducted under physiological conditions (pH 7.4) to examine controlled release behavior over time [4].

Conclusion

This study successfully synthesized and characterized PEG-coated Fe_3O_4 MNPs as a nanocarrier for dexamethasone. The nanoparticles exhibited well-defined morphology, effective PEG functionalization, and high drug-loading efficiency. Drug release studies revealed a sustained release profile, suggesting the potential of PEG-coated Fe_3O_4 MNPs for controlled drug delivery applications. These findings indicate that PEG-functionalized Fe_3O_4 MNPs could serve as a promising platform for targeted drug delivery, decreasing systemic side influences and enhancing therapeutic outcomes. Further in vitro and *in vivo* investigations are needed to validate their clinical applicability.

References

[1] S. Laurent *et al.*, “Erratum: Magnetic iron oxide nanoparticles: Synthesis, stabilization, vectorization, physicochemical characterizations, and biological applications (Chemical Reviews (2008) 108 (2064)),” *Chem. Rev.*, vol. 110, no. 4, p. 2574, 2010, doi: 10.1021/cr900197g.

[2] J. Xie, J. Huang, X. Li, S. Sun, and X. Chen, “Iron Oxide Nanoparticle Platform for Biomedical Applications,” *Curr. Med. Chem.*, vol. 16, no. 10, pp. 1278–1294, 2009, doi: 10.2174/092986709787846604.

[3] S. A. Gaballa *et al.*, “Corticosteroids in ophthalmology: drug delivery innovations, pharmacology, clinical applications, and future perspectives,” *Drug Deliv. Transl. Res.*, vol. 11, no. 3, pp. 866–893, 2021, doi: 10.1007/s13346-020-00843-z.

[4] Q. Zheng *et al.*, “Remote-controlled dexamethasone-duration on eye-surface with a micelle-magnetic nanoparticulate co-delivery system for dry eye disease,” *Acta Pharm. Sin. B*, vol. 14, no. 8, pp. 3730–3745, 2024, doi: 10.1016/j.apsb.2024.05.004.

[5] H. Veisi, S. B. Moradi, A. Saljooqi, and P. Safarimehr, “Silver nanoparticle-decorated on tannic acid-modified magnetite nanoparticles (Fe 3 O 4 @TA/Ag) for highly active catalytic reduction of 4-nitrophenol, Rhodamine B and Methylene blue,” *Mater. Sci. Eng. C*, vol. 100, no. December 2018, pp. 445–452, 2019, doi: 10.1016/j.msec.2019.03.036.

[6] A. H. Lu, E. L. Salabas, and F. Schüth, “Magnetic nanoparticles: Synthesis, protection, functionalization, and application,” *Angew. Chemie - Int. Ed.*, vol. 46, no. 8, pp. 1222–1244, 2007, doi: 10.1002/anie.200602866.

O18. Manufacturing and Optimization of the properties of Jute-Kevlar/Nano Fumed Silica hybrid reinforced epoxy composite using Taguchi technique

Sasidhar Pentapati *, Pramod Kumar Parida, Arun Kumar Pradhan
School of Mechanical Sciences, Indian Institute of Technology Bhubaneswar, Odisha, India
* *+919381621272, a24me09008@iitbbs.ac.in*

Natural fiber-based composites are in high demand due to their low cost and eco-friendly nature. The current study aims to create a sustainable and economical material by hybridizing affordable, biodegradable jute fiber with conventional high performance fibers. Extensive studies on the effects of various control parameters on the performance of Jute-Kevlar hybrid reinforced epoxy composites with fumed silica (NFS) nano-filler using Taguchi optimization technique is carried out. For this purpose four design parameters (fiber wt. %, filler wt.%, orientation and stacking sequence) at three levels were decided, accordingly orthogonal array L27 is chosen and a total of 27 composite laminates were fabricated. Tensile, flexural tests were then carried out on specimens to study the effect of various control factors on the properties of composites. Taguchi optimization technique enabled the determination of optimal control parameter settings. Using this maximization of tensile and flexural strength were achieved. ANOVA approach has been carried out to know the p-values of significant factors. Mathematical Model has been formulated by performing regression analysis. Confirmation test has been carried out at optimum conditions to know the reliability of mathematical model.

References

[1] Dawoud, Mohamed M., and Hosam M. Saleh. "Introductory chapter: Background on composite materials." Characterizations of Some Composite Materials. Intech Open (2018): 1-10.
[2] Sunil Manohar Maharana, Arun Kumar Pradhan & Mihir Kumar Pandit (2022) Performance Evaluation of Mechanical Properties of Nanofiller Reinforced Jute-Kevlar Hybrid Composite, Journal of Natural Fibers, 19:3, 984-998, DOI: 10.1080/15440478.2020.1777246
[3] Parida, P.K., Pentapati, S. & Pradhan, A.K. Thermomechanical Characterization of Myriostachya wightiana Stem Fiber (MWSF)/Epoxy Composite: A Sustainable Material. Mater Circ Econ 6, 22 (2024). https://doi.org/10.1007/s42824-024-00115-y

O19. Green synthesis of copper oxide nanocatalyst using plant extract and its antibacterial and photocatalytic applications

Ganesh Dawange, [1,2] Vikram Pandit[1] *

[1]*Haribhai V. Desai College, Pune, India*
[2]*Sanjivani College of Engineering, Kopargaon, India*
*Email: vikramupandit@gmail.com

Photocatalysis is one of the efficient methods applied for the treatment of wastewater. The CuO nanoparticle photocatalyst was synthesized using a leaf extract from a Mitragyna parviflora plant by the precipitation method, and its efficiency was assessed in the photocatalytic applications. The prepared CuO nanomaterials were characterized using XRD, FTIR, EDX, SEM and UV-Vis spectroscopy. The X-RD analysis showed CuO nanoparticles with monoclinic structure that have average crystalline sizes in the range of 25.3 to 10.5 nm. The FT-IR spectrum showed the stretching vibration bands typical of Cu-O bonds, and the optical band gaps were between 2.6 and 1.7 eV. Energy-dispersive X-ray (EDX) analysis of copper (Cu) nanoparticles typically reveals their elemental composition, confirming the presence of Cu. SEM imaging reveals the shape, size, and distribution of the nanoparticles. The catalytic efficiency of CuO nanoparticles using Mitragyna parviflora leaf extract was assessed for antibacterial activity against Escherichia coli, antibacterial activity against Pseudomonas aeruginosa, and antibacterial activity against Staphylococcus aureus. The degradation of methylene blue (MB) and organic matter is done by using different concentration amounts of CuO. The effect of different parameters, such as the concentration of CuO, pH, and concentrations of the (5, 10, 20, 50 ppm) MB solution, and the influence of sunlight radiation were examined.

O20. Green synthesis of silver nanoparticles of *Spondias Mombin* and *Terminalia Ivorensis* ethanolic extracts and investigation of their antimicrobial activities

David Adeyemi [1, *], Adebowale Adeluola[2], Precious Airuoyefe[1]
Modupe Ologunagba[2] Gloria Ayoola[1]

[1] Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Lagos, Nigeria
[2]Department of Pharmaceutics and Pharmaceutical Technology, Faculty of Pharmacy, University of Lagos, Nigeria
+234803387145, dadeyemi@unilag.edu.ng

Introduction

Recently, there have been increasing antibiotic resistance by microorganisms, posing serious health hazards to humans. Nanoparticles have proved to be a promising candidate as antimicrobial agent, since their large surface area to volume ratio ensures a broad range of attack on bacterial surface. The leaves of *Spondias mombin* (SM) extracts have been reported to possess anxiolytic, hypoglycaemic, antiepileptic, antipsychotic, sedative, antioxidant, and antimicrobial properties. Also, ethno-medicinally, the pulverized leaves of *Terminalia Ivoriensis* (TI) have been used as poultice in treatment of burns and bruises. The objective of this study was to determine the antibacterial potentials of silver and zinc nanoparticles (NPs) of the SM and TI aqueous leaves extract.

Method

NPs were synthesized from reactions of silver salts precursor and 50% ethanolic plant extracts at optimized conditions. NPs were characterized by UV-Visible, FT-IR and SEM analysis. Determination of the antimicrobial activities against isolated strains of gram positive and gram-negative bacteria was by agar well diffusion technique. The antibacterial activities were by measuring zone of inhibition (ZI) and minimum inhibitory concentration (MICs).

Results and discussion

The yield of NPS increases with the amount of precursor metal salt used in the synthesis. The optimal yield was 90 % for 3.0g of the $AgNO_3$. The derived NPs varied from dark brown to colorless and appears predominantly rod shape with size ranging from 65-120 nm. The UV-Vis absorption spectra of SM and TI AgNPs had maximum absorbance at wavelengths (λmax) of 267 and 262 nm respectively. The AgNPs exhibited lower energy absorption bands compared to the previous studies on crude extract. The FT-IR results shows that the phytochemicals in the plants acted as reducing and stabilizing agent during the NPs synthesis. The NPs exhibit dose-dependent antibacterial activities (15>10>5mg/ml). Both SM and TI nanoparticles inhibited 72.7% of microorganisms under study, and were more active on Gram -ve than Gram +ve bacteria. Levofloxacin standard exhibited similar activity on Gram +ve (ZI= 15.17-32.5mm) to Gram -ve (ZI=13.3-35.2mm) bacterial investigated. Also, the SM AgNPs showed similar ZI (1.2-20.7mm) when to TI AgNPs (1.20-20.3mm). The ZI of NPs were relatively lower when compared to levofloxacin standard (12.8-42.3 mm). The MICs of NPs (0.05-0.8 mg/ml) investigated in this study were higher than that of levofloxacin (50.0-6.3 µg/L).

Conclusion

This study confirms the potentials of green nanoparticles as alternative means for the development of novel antimicrobial agents for several clinical and biotechnological applications.

Keywords: Nanoparticles, FT-IR, antibacterial, inhibition.

References

Aromolaran, O., and Badejo, O. K. Efficacy of fresh leaf extracts of Spondias mombin against some clinical bacterial isolates from typhoid patients. Asian Pac J Trop Dis. 4: 442 – 446; 2014.

Patra S, Mukherjee S, Barui AK, Ganguly A, Sreedhar B and Patra CR. Green synthesis, characterization of gold and silver nanoparticles and their potential application for cancer therapeutic, Materials Science and Engineering 53: 298–309; 2015.

Palaniselvam, K., Mashitah, M. Y., Gaanty, P. M., and Natanamurugaraj, G. Biosynthesis of metallic nanoparticles using plant derivatives and their new avenues in Pharmacological applications – An updated report. Saudi Pharm J. 24: 473 484; 2016.

Adeyemi DK, Adeluola AO, Akinbile MJ, Johnson OO and Ayoola GA. Green synthesis of Ag, Zn and Cu nanoparticles from aqueous extract of Spondias mombin leaves and evaluation of their antibacterial activity. African Journal of Clinical and Experimental Microbiology 21 (2): 106-113, 2020.

Adeyemi D.K, Adeluola Adebowale, Johnson Oluwatosin, Giwa Mariam, Shonekan Omonike. Green Synthesis of Silver, Zinc and Copper Nanoparticles from aqueous extract of Terminalia Ivorensis (A. Chev.) leaves and their antimicrobial activities. African Journal of Pharmaceutical Research and Development 12(2):164-171; 2020

O21. Sustainable Adsorption of Congo Red Dye Using Natural Bentonite and Hydroxyapatite: Mechanistic Insights, Optimization, and Reusability

Ayoub Grouli, Nada El arrach, Houria Hamdani, Soumia Belouafa,
Mohammed Berrada
*Laboratory of Health and Biology (LBS), Faculty of Sciences Ben M'Sick, Department of Chemistry,
University Hassan II of Casablanca, Casablanca, 20000, Morocco*

Congo Red (CR), a toxic and carcinogenic dye, poses severe environmental and health risks. This study explores natural bentonite and hydroxyapatite (HA) as eco-friendly adsorbents for CR removal. Structural analysis via XRD confirmed their crystalline phases, while FTIR identified functional groups (e.g., hydroxyl, phosphate) involved in adsorption. SEM revealed porous morphologies, enhancing surface area for dye interaction. Optimization using the Box-Behnken design pinpointed ideal parameters: pH 6.5, 150 mg/L initial CR concentration, and 1.5 g/L adsorbent dosage, achieving 95% (HA) and 84% (bentonite) removal efficiencies. Monte Carlo simulations highlighted the spontaneity of adsorption, driven by van der Waals forces, with stronger affinity under acidic conditions due to favorable electrostatic interactions. Kinetic studies fit the pseudo-second-order model ($R^2 = 0.99$), suggesting chemisorption via surface bonding. Thermodynamic data indicated an exothermic, entropy-driven process. Reusability tests using desorption agents (e.g., ethanol) demonstrated HA and bentonite retained 75% and 60% efficiency, respectively, after five cycles, underscoring their durability. HA's superior performance stems from its higher surface reactivity and ion-exchange capacity. The cost-effectiveness, abundance, and minimal environmental footprint of these adsorbents make them viable for industrial wastewater treatment. This work elucidates adsorption mechanisms, emphasizing the role of material structure and environmental factors, while advocating sustainable solutions to combat dye pollution. By bridging experimental and computational insights, the study advances practical strategies for eco-remediation, aligning with global goals for cleaner water systems and reduced chemical hazards.

References

[1] Grouli, A.; Chraka, A.; Bachra, Y.; Elkouali, M.; Chtita, S.; Berrada, M. An Investigation of the Adsorption of Congo Red Dye on Two Naturally Occurring Adsorbents Hydroxyapatite and Bentonite: An Experimental Analysis, DFT Calculations, and Monte Carlo Simulation. Heliyon 2024, 10,

[2] Fouad, D.; Bachra, Y.; Ayoub, G.; Ouaket, A.; Bennamara, A.; Knouzi, N.; Berrada, M. A Novel Drug Delivery System Based on Nanoparticles of Magnetite Fe 3 O 4 Embedded in an Auto Cross-Linked Chitosan. In Chitin and Chitosan - Physicochemical Properties and Industrial Applications [Working Title]; IntechOpen, 2020.

O22. Zeta Potential and Particle Size Investigation on Bentonite Activation

Burak ÜNLÜ *, Serbülent TÜRK

Sakarya University, Biomedical, Magnetic and Semiconductor Materials Research Center (BIMAS-RC), 54187, Sakarya, Turkey

* *+90 264 295 31 71, burakunlu@sakarya.edu.tr*

Bentonite is a clay material that contains a montmorillonite structure. The montmorillonite crystal structure is dioctahedral; trivalent cations occupy two-thirds of octahedral sites. The generally accepted structured formula of montmorillonite is $M^{+}_{y}.nH_2O(Al_{2y}, Mg_y)Si_4O_{10}$ M is a cation. Structure charges of dioctahedral montmorillonite originated from the substitution of Mg2+ for Al3+ in an octahedral sheet [1]. Activation is a treatment that can be chemical or physical to increase reactivity. For clays, activation has been used to increase the capacity of adsorption of coloring matter or some impurities in oils and solutions [2]. In this study, bentonite powder was activated by sodium hydroxide, hydrochloric acid and sodium chloride. Activated bentonite samples were investigated using Zeta Potential and DLS methods.

References

[1] S. F. A. Shattar, N. A. Zakaria, and K. Y. Foo, “One step acid activation of bentonite derived adsorbent for the effective remediation of the new generation of industrial pesticides,” *Sci Rep*, vol. 10, no. 1, Dec. 2020, doi: 10.1038/s41598-020-76723-w.

[2] H. Babaki, A. Salem, and A. Jafarizad, “Kinetic model for the isothermal activation of bentonite by sulfuric acid,” *Mater Chem Phys*, vol. 108, no. 2–3, pp. 263–268, Apr. 2008, doi: 10.1016/j.matchemphys.2007.09.034.

O23. Metal loaded 6,13-Pentacenequinone and 5, 7, 12, 14-Pentacenetetrone for Photocatalytic Applications

Sakshi Thombare, [a,b], Harsh Gaikwad, [a] Dalila Hammichhe,[c] Vikram Pandit[b]

[a] *Department of Chemistry, PES's Modern College of Arts, Science & Commerce, Pune-05, India*

[b] *Haribhai V. Desai College, Pune-02, India*

[c] *Bejaia University, Bejaia, Algeria*

In the past, many researchers have reported inorganic semiconductor oxide, sulfide systems, and nanocomposites as a photocatalyst for hydrogen production as well as dye degradation. Recently, the use of graphene, carbon nanotubes, and conducting polymers along with metal oxides as good photocatalytic materials has been reported. Organic solar cells, OFET and organic light-emitting diodes[14] are some excellent applications where pentacene is mostly used. Organic semiconductors have several advantages: (a) low cost synthesis and (b) easy manufacture of thin film devices by vacuum evaporation/sublimation or solution cast or printing technologies. Pentacene is a benchmark organic semiconductor in thin-film organic electronic devices due to its π-conjugated electronic structure, its relatively low HOMO-LUMO gap and the relatively high charge carrier mobility of its solid state films. Various methods are there to synthesize 6,13-Pentacequinone(PQ) and 5,7,12,14-Pentacetetrone(PT). Synthesis of 6,13-Pentacequinone from o-Phathaldehyde and 1,4-Cyclohexadione using potassium hydroxide. Also, Synthesis of 5,7,12,14-Pentacetetrone from 2-methyl-1,4-naphthoquinone and N-methylcyclohexylamine using ethanol. We believe that, these compounds when loaded with transition metals then they may found photocatalytic activeness.

O24. Design of $SrTiO_3$-Based Thermoelectric Composites with In Situ Exsolved Mo–Ni Alloys for Enhanced Performance

Miguel A. Vieira[1*], Aleksey. A. Yaremchenko[1], Wenjie Xie[2,3], Anke Weidenkaff[2,3], Andrei. V. Kovalevsky[1]

[1]CICECO – Aveiro Institute of Materials, Department of Materials Engineering and Ceramics (DEMaC), University of Aveiro, 3810-193, Aveiro, Portugal

[2]Materials and Resources, Department of Materials and Earth Sciences, Technical University of Darmstadt, Darmstadt 64287, Germany

[3]Fraunhofer Research Institution for Materials Recycling and Resource Strategies IWKS, Alzenau 63755, Germany

[*]916581218, *miguelamado@ua.pt*

With the increasing demand for sustainable energy sources, thermoelectric materials, which convert waste heat into electricity, are emerging as a promising solution for energy recovery. Most oxides are not suitable for thermoelectric (TE) heat harvesting due to low ZT values when compared with traditional TE, but new compositions, microstructures, and processing techniques can enhance performance [1,2]. Among promising oxide materials for TE applications, $SrTiO_3$-based ceramics are particularly appealing due to their sensitivity to redox and processing conditions, enabling tunable electrical and thermal properties [3]. This work explores the new design principles for such materials by combining a model Pr-substituted $SrTiO_3$ ceramics with, in situ exsolved $MoNi_4$ intermetallic micro- and nanoparticles. The resulting composites were analysed to assess their thermoelectric performance and potential for waste heat recovery. X-ray diffraction (XRD) and Scanning electron microscopy (SEM) confirmed that the ceramics matrix had a single-phase perovskite structure and revealed that the $MoNi_4$ nanoparticles were well-dispersed within the matrix. The Seebeck coefficient was found to be slightly lower compared to the unmodified matrix, as expected with nanoparticle incorporation. Electrical conductivity measurements showed a notable improvement, attributed to enhanced charge carrier transport. As a result, an attractive power factor value was obtained at 1173 K, reaching a value of 1180 uW/m·K^2, demonstrating a clear improvement over the matrix. Due to the minor variations in thermal conductivity for the low $MoNi_4$ content range, the maximum ZT reaches 0,32 at 1173 K. The current results highlight the potential of $Sr_{0.9}Pr_{0.1}TiO_3$-$MoNi_4$ composites for efficient waste heat recovery using thermoelectric effect.

References

[1] A. V. Kovalevsky, K. V. Zakharchuk, M.H. Aguirre, W. Xie, S.G. Patrício, N.M. Ferreira, D. Lopes, S.A. Sergiienko, G. Constantinescu, S.M. Mikhalev, A. Weidenkaff, J.R. Frade, Redox engineering of strontium titanate-based thermoelectrics, Journal of Materials Chemistry A. 8 (2020) 7317–7330

[2] M. Backhaus-Ricoult, J. Rustad, L. Moore, C. Smith, J. Brown, Semiconducting large bandgap oxides as potential thermoelectric materials for high-temperature power generation?, Appl. Phys. A Mater. Sci. Process.116 (2014) 433–470

[3] X. L. Shi, H. Wu, Q. Liu, W. Zhou, S. Lu, Z. Shao, M. Dargusch, Z. G. Chen, SrTiO3-based thermoelectrics: Progress and challenges, Nano Energy. 78 (2020)

O25. Nanoplastics Fragmentation and Characterization Using a Solvent-Free Method

Emmanuel S.C. Miguel *, Priscila S. Cavalheri, Anderson R.L. Caires
Institute of Physics, Federal University of Mato Grosso do Sul, Av. Costa e Silva, s/nº Campo Grande, MS, Brazil
* *+55(67)3346-9876, engesc.miguel@gmail.com*

Abstract

A detailed characterization of nanoplastics (NPs) is crucial for assessing environmental risks and interactions with organisms. In this study, a mechanical method based on high-frequency ultrasound was adapted to obtain plastic nanoparticles without the use of solvents such as toluene. This cavitation-based approach enabled the fragmentation of plastic pellets into nanofilms and nanoparticles with a well-defined size distribution, as confirmed by scanning electron microscopy (SEM) and dynamic light scattering (DLS). Unlike standardized laboratory approaches that rely on model nanoparticles, this method utilizes commercially available plastic from industrial processes, ensuring greater environmental representativeness of the generated fragments. The results highlight the efficiency and advantages of cavitation as an alternative technique for obtaining plastic nanoparticles, providing valuable insights for future studies on their environmental behavior and potential impacts.

Introduction

Plastic pollution in aquatic environments remains a significant issue due to the slow degradation of plastics and their potential ecological impacts. A major challenge in studying plastic nanoplastics is their colloidal stability, as pH-dependent surface charges promote aggregation, affecting dispersion and bioavailability [1].

This study presents a solvent-free mechanical method for obtaining plastic nanoparticles, which can be applied to different polymeric materials. High-density polyethylene (HDPE) was selected as a model due to its high mechanical resistance and environmental persistence, making it one of the most challenging plastics to degrade. Using scanning electron microscopy (SEM), dynamic light scattering (DLS), and Fourier-transform infrared spectroscopy (FTIR), the morphology, size distribution, and chemical composition of the particles are analyzed, providing essential insights into their environmental behavior and potential impacts.

Method

The initial phase of this study involved obtaining and preparing nanoparticles of HDPE from industrial recycled pellets (~5 mm in diameter). The pellets were initially fragmented using a knife mill, significantly reducing the particle size. To achieve nanoscale particles, pre-fragmented material was dispersed in distilled water (1:1 m/m) and sonicated in pulsed mode using a high-frequency ultrasonic processor operating at 14 kHz. To prevent reagglomeration, the process was conducted in an ice-water bath at 0°C.

The samples were then washed and filtered using 0.20 µm membrane filters, ensuring sample homogeneity for further analysis. The samples were characterized using Dynamic Light Scattering (DLS) and Zeta Potential measurements to assess nanoparticle formation and colloidal stability. Scanning Electron Microscopy (SEM) provided morphological analysis, while Fourier Transform Infrared Spectroscopy (FTIR) confirmed the chemical composition of HDPE.

Results

DLS analysis revealed that approximately 60% of the sample had an average hydrodynamic diameter of 100 nm (Figure 1a). The morphology of the particles, analyzed by SEM (Figures 1b), showed irregular surfaces, typical of materials fragmented by ultrasonic cavitation.

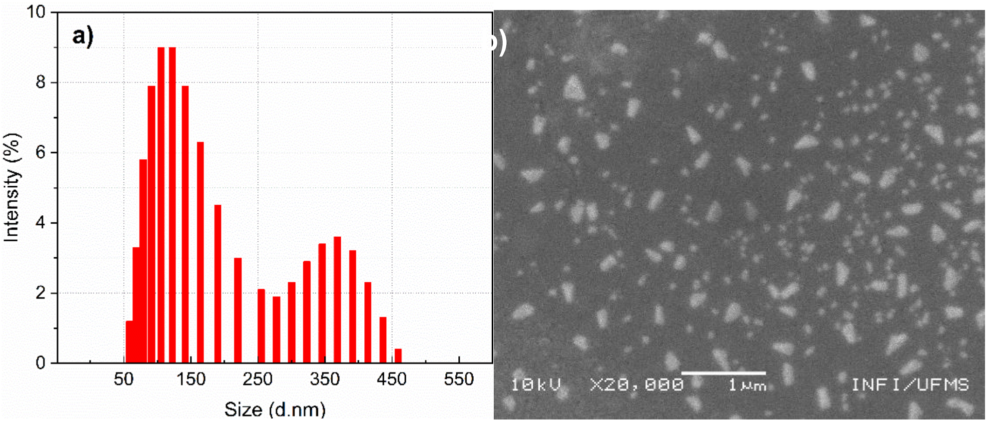


Figure 1 - a) Particle Size Distribution Obtained by DLS, b) SEM Image at 20,000× Magnification.

The FTIR spectrum (Figure 2a) confirmed the chemical identity of HDPE, exhibiting characteristic vibrational bands, including CH_2 peaks at 2915 cm^{-1}, 2848 cm^{-1}, 1465 cm^{-1} and 720 cm^{-1}. Among these, the band at 720 cm^{-1} stands out as a strong identifying feature of HDPE [2].

The mean zeta potential (Figure 2b) of -15.5 mV indicates moderate colloidal stability, influenced by the low density of ionizable charges on the polymer surface [1]. Its low polarity reduces electrostatic stabilization in aqueous media, favoring particle aggregation [3].

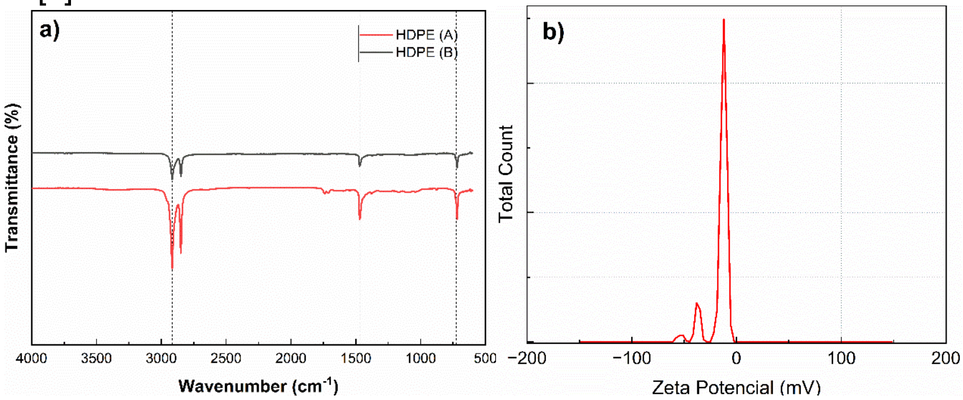


Figure 2 - a) FTIR Spectra of HDPE: (A) Fragmented plastics and (B) Pristine HDPE Pellets, b) Zeta Potential Distribution of Nanoparticles.

Discussion

The sonication method effectively fragmented HDPE into nanoparticles without the use of solvents, generating environmentally relevant nanoplastics. The cavitation process not only enabled size reduction but also preserved the polymer's chemical integrity, as evidenced by the absence of oxidative degradation. This is crucial because degraded plastics often exhibit altered surface properties, which can influence their interactions with environmental contaminants and biological systems [4]. This solvent-free approach ensures that the generated nanoplastics closely resemble real-world contaminants, making them ideal for ecotoxicological studies [5].

Future research will focus on assessing the toxicity of these nanoplastics using bioindicators from different trophic levels. This will provide valuable insights into their bioavailability, uptake, and potential risks to aquatic organisms, contributing to a more comprehensive understanding of nanoplastic pollution and its ecological consequences.

References

[1] T. Cao, M. Zhao, T. Zhang, and W. Chen, *Environ Sci Nano*, **12**, 232–240, (2025).
[2] J. Charles and G. R. Ramkumaar, *Asian J. Chem.*, **21**, 4477–4484 (2009).
[3] S. Seidensticker, P. Grathwohl, J. Lamprecht, and C. Zarfl, *Environ Sci Eur*, **30**, 1–12, (2018).
[4] A. A. Cuadri and J. E. Martín-Alfonso, *Polym Degrad Stab*, **141**, 11–18, (2017).
[5] S. Ducoli, G. Kalčíková, M. Velimirovic, L. E. Depero, and S. Federici, Environ. Chem. Lett., **23**, 649–675, (2025).

O26. Synthesis and Characterization of Polymer Nanoparticles Loaded with Lapachol for Biomedical Applications

Maria Victória Pereira Dias *, Regiane Godoy de Lima,
Anderson Rodrigues Lima Caires
Optics and Photonics Group, Institute of Physics, Federal University of Mato Grosso do Sul, P.O. Box 549, 79070-900 Campo Grande, MS, Brazil
**+55 11 97317-7342, m.victoria@ufms.br*

In recent years, nanoparticles have emerged as a promising approach for various scientific and technological applications, especially in the biomedical field.[1] These structures have nanometre-scale dimensions, conferring unique properties such as greater surface area, better solubility and greater reactivity compared to their micro- or macro-scale counterparts. Lapachol, a natural compound extracted from trees of the Tabebuia genus, has relevant pharmacological properties, including anticancer, antimicrobial and antioxidant activity.[3] However, its low water solubility and limited bioavailability pose challenges to its clinical use. Incorporating Lapachol into nanoparticles has emerged as a viable strategy to optimise its physicochemical properties, improve its absorption and reduce possible adverse effects. This study aims to synthesise and characterise Lapachol nanoparticles using the nanoprecipitation technique. Different analytical techniques such as UV-Vis spectroscopy, absorbance, scanning electron microscopy (SEM) and nanotoxicity tests were used to assess the stability, morphology and safety of the synthesised nanoparticles. Lapachol nanoparticles were synthesised using the nanoprecipitation technique, an efficient method for obtaining homogeneous and stable particles.[2] Characterisation was carried out using different analytical techniques, including UV-Vis spectroscopy, absorbance, scanning electron microscopy (SEM) and nanotoxicity tests. UV-Vis spectroscopy revealed characteristic Lapachol bands, indicating that the compound's structure was preserved after nanoencapsulation. Absorbance tests showed good colloidal stability of the nanoparticles in solution. Morphological analysis by SEM confirmed the formation of spherical nanoparticles with uniform size distribution. In nanotoxicity tests, the nanoparticles showed low toxicity to human cells at moderate concentrations, suggesting their viability for biomedical applications. However, at higher doses, cytotoxic effects were observed, highlighting the importance of precise concentration control for future therapeutic applications. The characterisation of Lapachol nanoparticles showed the effectiveness of the nanoprecipitation technique in obtaining homogeneous and stable particles. The combination of different analytical methods enabled a detailed assessment of their properties, contributing to the development of promising nanotechnological formulations in the biomedical and pharmaceutical fields.

References

[1] Ferreira, Hadma Sousa, e Maria do Carmo Rangel, Nanotecnologia: aspectos gerais e potencial de aplicação em catálise, *Química Nova*, vol. 32, 2009, p. 1860–70.
[2] Lima, Regiane G., et al, Preparation and Phytotoxicity Evaluation of Cellulose Acetate Nanoparticles, *Polymers*, vol. 14, nº 22, 2022, p. 5022.
[3] H. Hussain, K. Krohn, V. U. Ahmad, G. A. Miana and I. R. Green, Lapachol: An overview, Arkivoc, 2007, 2007, 145–171

O27. Determination of Photosensitizing Potential of Lapachol for Photodynamic Inactivation of Bacteria

Regiane G. Lima*, Raphael S. Flores, Gabriella Miessi, Jhoenne H. V. Pulcherio, Laís F. Aguilera, Leandro O. Araujo, Samuel L. Oliveira, Anderson R. L. Caires
Optics and Photonics Group, Institute of Physics, Federal University of Mato Grosso do Sul, P.O. Box 549, 79070-900 Campo Grande, MS, Brazil
* *+55 (18) 991146626, regiane.godoy@ufms.br*

Antimicrobial resistance is a global health crisis, driving the search for alternative therapies such as antimicrobial photodynamic inactivation (aPDI), which combines a photosensitizer (PS), light, and oxygen to generate reactive oxygen species (ROS) that kill bacteria. In this context, the present study evaluated lapachol, a natural naphthoquinone extracted from *Tabebuia avellanedae*, as a potential PS for aPDI against *Staphylococcus aureus* and *Escherichia coli*. Lapachol was optically characterized by UV-vis spectroscopy, revealing two prominent absorption bands at 280 and 482 nm, with the latter suitable for activation with blue light (450 nm). The ROS-generating ability of lapachol under blue LED exposure was assessed using dihydroethidium (DHE), confirming time-dependent fluorescence emission due to ROS formation. Antibacterial assays were performed using increasing concentrations of lapachol (6,25–25 $\mu g\cdot mL^{-1}$) in both irradiated and dark conditions. *S. aureus* was completely inactivated at 25 $\mu g\cdot mL^{-1}$ with an energy dose of 100 $J\cdot cm^{-2}$, while *E. coli* showed a limited two-log reduction under higher energy (150 $J\cdot cm^{-2}$), likely due to its protective outer membrane. Scanning electron microscopy (SEM) revealed intact morphology in non-irradiated controls and significant structural damage, including membrane disruption and lysis, in irradiated bacteria[1]. These findings demonstrate lapachol's selective photodynamic activity and low dark toxicity, reinforcing its potential as a natural, visible-light-activated photosensitizer. This work contributes to the growing field of plant-based phototherapeutics for bacterial control. For reference, similar quinone-based PSs have shown promise in cancer PDT applications[2], and recent nanocarrier formulations combining lapachol with other photosensitizers have improved ROS stability and therapeutic efficacy[3]. Overall, lapachol presents as a promising candidate for topical aPDI applications, especially against Gram-positive bacteria.

References

[1] Lima, R.G. et al., *Molecules*, 29, 5184 (2024).
[2] Rajendran, M., *Photodiagn. Photodyn. Ther.*, 13, 175–187 (2016).
[3] Campanholi, K.S.S. et al., *Dyes and Pigments*, 157, 238–250 (2018).

O28. Graphitic Carbon nitride: Effect of various precursors on dye degradation and drug degradation

Tushar Patil [a], Vikram Pandit, [b] * Vijaykumar Chavan [a]

[a] *Dr. Yusuf Hamied Department of Chemistry, Ramnarain Ruia Autonomous College, Mumbai 400019, India*

[b] *Department of Chemistry, Haribhai V. Desai College of Arts, Science & Commerce, Pune-411002, India*

Email: vikramupandit@gmail.com

This study explores the potential of graphitic carbon nitride (g-C3N4) with various precursors (Melamine, Urea, Thiourea) for photocatalytic applications. Initially graphitic carbon nitride nanostructures were synthesized with thermal polymerization method. FESEM and TEM surface morphology. XRD confirmed their crystalline structure, while UV-Vis spectroscopy indicated a bandgap of 2.8 eV (absorption at 380 nm). Increasing reaction parameters induced morphological evolution into three-dimensional distorted spherical structures. Photocatalytic evaluation under UV light demonstrated superior degradation of Rhodamine 6G (R6G) by the 5 wt.% Ag-ZnO composites, achieving 93.36% efficiency with a rate constant of 6.54×10^{-3} min^{-1}. This composite also exhibited remarkable recyclability, retaining >91% activity after five cycles. Antioxidant assessments (DPPH, ABTS, FRAP, FIC) highlighted the 5 wt.% Ag-ZnO's exceptional radical scavenging capacity, underscoring its dual functionality.

O29. Synthesis, characterization, and evaluation of cellulose acetate nanoparticles as a photosensitizing agent in photodynamic inactivation against S. aureus and E. coli bacteria

Raphael de S. Flores *, Regiane G. Lima, Gabriella M. Campos,
Anderson R. L. Caires
Instituto de Física – Universidade Federal de Mato Grosso do Sul
* *+55 67 984799 5580, raphael.rflores@gmail.com.*

Throughout history, humanity has faced a variety of diseases caused by bacterial infections. The discovery of antibiotics transformed modern medicine and significantly increased life expectancy. However, the improper and excessive use of these medications over the years has contributed to an alarming rise in bacterial resistance. One strategy that has proven effective in eradicating microorganisms is photodynamic inactivation (PDI). Given this, the present study aimed to synthesize and characterize cellulose acetate nanoparticles (CAt-NPs) using the organic compound THF as a solvent (CAt-NPs) and to evaluate their efficacy in the PDI process. The CAt-NPs were synthesized via the nanoprecipitation method and characterized by scanning electron microscopy (SEM), dynamic light scattering (DLS), Zeta potential, and FTIR. In the biological assays, strains of *Staphylococcus aureus* (*S. aureus*) ATCC 25923 and *Escherichia coli* (*E. coli*) ATCC 25922 were used, divided into two groups: (I) irradiated group and (II) non-irradiated group. The internalization time of the NPs was 1 hour, followed by an exposure of 1.5 hours to blue LED light with a wavelength of 450 nm and an energy dose of 28.84 $mW.cm^{-2}$ for the irradiated group. The concentrations tested for PDI were 100 ppm, 250 ppm, 500 ppm, and 1000 ppm of CAt-NPs. Biological tests indicated that CAt-NPs exhibit bactericidal effects at the higher concentrations against *E. coli* bacteria, whereas no significant effects were observed against S. aureus at any concentration.

References

[1] A. ARIAS, C.; E. MURRAY, B. Antibiotic-Resistant Bugs in the 21st Century - A Clinical Super Challenge. **The New England Journal of Medicine**, v. 360, p. 439–443, 2009.
[2] DEMIDOVA, T. N.; HAMBLIN, M. R. Effect of cell-photosensitizer binding and cell density on microbial photoinactivation. **Antimicrobial Agents and Chemotherapy**, v. 49, n. 6, p. 2329–2335, jun. 2005.

O30. Ag-Embedded Composites Ag-ZnO Nanostructures for Sustainable Solutions: Synergistic Photocatalytic Degradation and Antioxidant Efficacy

Vivekanand Jawale [a] [*], Vikram Pandit [b] [*]

[a] *Department of Chemistry, Modern College of Engineering Shivajinagar, Pune-411005, India*
[b] *Department of Chemistry, Haribhai V. Desai College of Commerce, Arts and Science, Pune-411002, India*

*Emails: vivekjawale25@gmail.com, vikramupandit@gmail.com

This study explores the dual-functional potential of silver-embedded zinc oxide (ZnO) nanocomposites with varying silver content (1, 3, and 5 wt.%) for enhanced photocatalytic and antioxidant applications. Initially, pure ZnO nanostructures were synthesized under controlled reaction parameters, revealing hexagonal rod-like morphologies via FESEM and TEM analyses. XRD confirmed their crystalline wurtzite structure, while UV-Vis spectroscopy indicated a bandgap of 3.27 eV (absorption at 380 nm). Increasing reaction parameters induced morphological evolution into three-dimensional distorted spherical structures. Photocatalytic evaluation under UV light demonstrated superior degradation of Rhodamine 6G (R6G) by the 5 wt.% Ag-ZnO composite, achieving 93.36% efficiency with a rate constant of 6.54×10^{-3} min^{-1}. This composite also exhibited remarkable recyclability, retaining >91% activity after five cycles. Antioxidant assessments (DPPH, ABTS, FRAP, FIC) highlighted the 5 wt.% Ag-ZnO's exceptional radical scavenging capacity, underscoring its dual functionality.

O31. Raman spectroscopy study of structural transformations in van der Waals ferrielectric CuInP2S6

A. Kohutych, M. Medulych, V. Hryts, M. Pop, V. Liubachko, A. Pogodin,
R. Yevych, K. Glukhov, **Yu. Vysochanskii** *
Institute for Solid State Physics and Chemistry, Uzhhorod National University, Uzhhorod, Ukraine
* *vysochanskii@gmail.com*

The appearance of spontaneous polarization in van der Waals (vdW) $CuInP_2S_6$ ferrielectrics is related to the second order Jahn-Teller effect for copper cations located in a double-well local potential, and to the stereoactivity of indium cations located in a three-well local potential. A molecular dynamics simulation demonstrated these peculiarities of chemical bonds [1]. The ferrielectric phase transition can be described using the mixed Ising model [2] with pseudospins $s = ½$ (Cu^+ cations flipping) and $S = 1$ (In^{3+} cations displacements). The calculated pseudospin fluctuation spectrum shows that the lattice anharmonicity is determined by the indium sublattice below 200 K, which induces the coexistence of the dipole glass and ferrielectric states [3]. Thermal activation of the copper relaxation dynamics results in the formation of a long-range fluctuating clusters of spontaneous polarization, even above the transition temperature into the paraelectric phase. The relaxation dynamics of Cu^+ cations is associated with significant deformations of the $(P_2S_6)^{4-}$ anions, causing buckling of the sulfur sheets [4]. The resulting rise in entropy from such structural disorder promotes the Cu^+ cations localization inside the vdW gap, where they bond to sulfur atoms from the neighboring structural layer. Formation of unfilled sulfide octahedra can also lead to the collinear orientation of the electric dipoles of In^{3+} and Cu^+ cations, inducing a crossover from the ferrielectric to the ferroelectric state. Raman spectroscopy revealed a softening of the low frequency spectral lines associated with the fluctuations of the indium cationic sublattice below 200 K as well as broadening of the spectral lines on heating due to disordering of the copper sublattice.

Acknowledgment: This work has been supported by the Horizon Europe Framework Programme, project no. 101131229, Piezoelectricity in 2D-materials: materials, modeling, and applications (PIEZO 2D).

References

[1] Yu. Vysochanskii, V. Liubachko, K. Glukhov, R. Yevych, A. Kohutych, V. Hryts, A. Dziaugys, J. Banys, *Ferroelectrics,* **618**, 906 (2024).
[2] W. Selke and J. Oitmaa, *J. Phys.: Condens. Matter.*, **22**, 076004 (2010).
[3] R. Yevych, V. Liubachko, V. Hryts, M. Medulych, A. Kohutych, Y. Vysochanskii, *Condensed Matter Physic*s, **27**, 14701 (2024).
[4] H. Luo e.a., *PNAS*, **121**, e2416835121(1-7) (2024).

O32. New Type Aortic Valve Design: Enhancing Surface Properties with Biofunctional Polymer Coatings

Rabia Güzide AL[1,2,*], Serbülent TÜRK[3], Hamid ASADI DERESHGI[4]

[1] *Biomedical Engineering, Institute of Natural Sciences, Sakarya University, Esentepe Campus, 54187 Sakarya, Türkiye* https://ror.org/04ttnw109

[2] *Department of Electronics and Electronic Engineering, Dogus University, 34775 Istanbul, Turkey* https://ror.org/0272rjm42

[3] *Biomedical, Magnetic and Semi Conductive Materials Research Center (BIMAS-RC), Sakarya University, Esentepe Campus, 54187 Sakarya, Türkiye* https://ror.org/04ttnw109

[4] *Department of Biomedical Engineering, Istanbul Arel University, 34537 Istanbul, Turkey* https://ror.org/03natay60

It remains a significant global health concern that valvular heart disease (VHD) affects more than one hundred million people and contributes markedly to cardiovascular morbidity and mortality. In developed countries, aortic stenosis represents the most prevalent indication for surgical intervention among patients with valvular disorders, reflecting its dominant clinical and epidemiological significance within this population [1]. There are primary surgical treatment options involving mechanical and bioprosthetic heart valves. Mechanical valves offer extended durability; however, their use is associated with an increased risk of thrombosis, necessitating lifelong anticoagulation therapy. In contrast, bioprosthetic valves offer improved hemodynamics and lower thrombogenicity, although their durability is limited by structural degeneration [2].

In this study, the surface properties of polymer-coated materials were investigated for potential use in heart valve applications. There were cycloaliphatic resin (CRS) samples coated with various polymer formulations, and their structural and chemical properties were assessed using surface characterization techniques. Scanning Electron Microscopy (SEM) was used to examine surface morphology, Energy Dispersive X-ray Spectroscopy (EDS) to determine elemental composition, Fourier Transform Infrared Spectroscopy (FTIR) to analyze chemical bonding, and contact angle measurements to evaluate surface wettability. The results demonstrated that polymer coatings, particularly those based on PVA-Chitosan, significantly enhanced surface smoothness, chemical interaction, and hydrophilicity, essential factors for biocompatibility.

Improving the surface characteristics of heart valve materials is essential for minimizing complications, such as thrombosis and blood cell damage, post-implantation. A more hydrophilic and chemically stable surface may reduce the risk of clot formation and improve the interaction between the material and blood. Consequently, polymer coatings provide a promising and effective strategy for advancing the development of safer, more biocompatible, and durable heart valve prostheses.

“Acknowledgement
This work was supported by the Scientific Research Projects Commission of Sakarya University (Project Number: 2024-26-62-63).”

References

[1] Iung, B., & Vahanian, A. (2011). Epidemiology of valvular heart disease in the adult. Nature Reviews Cardiology, 8(3), 162-172.

[2] Sun, J. C., Davidson, M. J., Lamy, A., & Eikelboom, J. W. (2009). Antithrombotic management of patients with prosthetic heart valves: current evidence and future trends. *The Lancet*, *374*(9689), 565-576.

O33. Effect of LiCl and CaCl2 Concentration on Physicochemical Properties of Sodium Alginate- Based Hydrogel

Merve KEYF[1,*], Serbülent TÜRK[2], Burak ÜNLÜ[2], Güler Bengüsu TEZEL[3]
[1] *Sakarya University, Biomedical Engineering, Institute of Natural Sciences, Esentepe Campus, 54187, Sakarya, Turkey*
[2] *Sakarya University, Biomedical, Magnetic and Semiconductor Materials Research Center (BIMAS-RC), 54187, Sakarya, Turkey*
[3] *Bolu Abant Izzet Baysal University, Faculty of Engineering, Department of Chemistry Engineering, Golkoy Campus, 14030, Bolu, Turkey*
[*] *+90 (545) 285 09 84, mervekeyf421@gmail.com*

Hydrogels based on natural polymers such as sodium alginate have received increasing attention in biomedical engineering due to their biocompatibility, non-toxicity, and adjustable physicochemical properties. In this study, sodium alginate-based hydrogels were synthesized using two different ionic crosslinking agents, LiCl and $CaCl_2$, and their impacts on the structural and functional characteristics of the hydrogels were investigated in detail. The aim of this research is to determine the most suitable hydrogel composition for potential applications in drug delivery and tissue engineering.

Hydrogels were prepared by dissolving 2.5% (w/v) sodium alginate in distilled water and crosslinked with varying concentrations of LiCl (0.5%, 1%, and 2%) and $CaCl_2$ (0.5%, 1%, and 2%). The mixtures were stirred at 300–400 rpm under regulated conditions and then poured into petri dishes for gelation. The hydrogels were then characterized in terms of swelling behavior, mechanical properties, and visual homogeneity. Preliminary results indicate that Ca^{2+} crosslinked hydrogels exhibit higher structural integrity and lower swelling ratios. [1] while Li^+ crosslinked samples showed greater flexibility and higher water uptake. [2]

This comparative approach provides new insightsand highlights the potential of adjusting hydrogel characteristics based on the type of crosslinker used. The results may guide the design of ionically adjustable hydrogel matrices suitable for controlled drug release or soft tissue scaffolding, particularly in systems where mechanical flexibility or ionic sensitivity is critical.

References

[1] Geyik, E. (2023). *Formulation and in vitro evaluation of sustained release calcium alginate beads of nifedipine*.
[2] Liu, Y. et al. (2023). *Sodium Alginate-Based High Conductive, Ultra-Stretchable Hydrogel Fibers for Electrolytes of Flexible Solid-State Supercapacitors*.

O34. Rheological Behavior of Natural Rubber Modified with Industrial Herbal Dust Ash

Teodora Vukša[*], Oskar Bera, Jelena Lubura Stošić
University of Novi Sad, Faculty of Technology Novi Sad, Bulevar cara Lazara 1, 21000 Novi Sad, Serbia
[*] *+381603039097; +38121450413, teodora.vuksa@gmail.com*

As tea is one of the most widely consumed beverages worldwide, there is a rising demand for this product. And with increasing filter tea production, there is a need for proper waste disposal, which comes as a result of the production process, and has numerous negative effects on the environment. A possible solution could be found in incorporating herbal dust ash into rubber products, as a more economic and environmentally friendly option. Rubber is a material with various applications of its products, due to its mechanical properties. Mostly used in clothing and automotive industry, rubber is a highly used product, and with this comes a need to make the production process more sustainable. Herbal dust ash, created by annealing herbal dust of green tea (*camellia sinensis*), hibiscus (*rosa sinensis*) and lemongrass (*melissa officinalis*) in a furnace with circulating air at 800 °C, was incorporated into the rubber mixture as filler, at 2.5 phr and 5 phr. The impact of this addition on rheological properties of the rubber mixture was examined. Results showed that the degree of chemical crosslinking of vulcanized samples with added herbal dust ash was similar with all herbal dust ash contents, and slightly lower than in samples without added ash. Cure rate index and optimal curing time showed minimal changes with the addition of herbal dust ash. These results indicate that adding herbal dust ash into rubber mixture does not significantly impact its rheological properties, therefore making this addition an important possibility for a more eco-friendly rubber industry.

O35. Investigation of Thermal Conductivity in Ethylene Glycol-Based Nanofluids Containing Er_2O_3 and Co_3O_4 Nanoparticles

Monther Alsboul[1,*], Mohd Sabri Mohd Ghazali[2], Mohamed R. Gomaa[3], Aliashim Albani[4]

[1]*Physics Department, College of Science, Al Hussein Bin Talal University, Jordan*

[2]*School of Fundamental Science, Universiti Malaysia Terengganu, Malaysia*

[3]*Mechanical Engineering Department, Faculty of Engineering, Al Hussein Bin Talal University, Jordan*

[4]*Renewable Energy & Power Research Interest Group (REPRIG), Eastern Corridor Renewable Energy (ECRE), Faculty of Ocean Engineering Technology and Informatics, Universiti Malaysia Terengganu, Malaysia*

[*] *+962772840300, +962 32179050, M.Alsboul@ahu.edu.jo*

Ethylene glycol is a widely utilized chemical in many industrial demands. The current study investigates the effect of adding Er_2O_3 -based Ethylene glycol and Co_3O_4 -based Ethylene glycol nanofluid on thermal conductivity. The effects of nanoparticle concentration at different solid volume fractions (0, 0.0625, 0. 125, 0.25, and 0.5%) were examined at a temperature range of 20-50 ºC. A magnetic stirrer and ultrasonic homogenizer were used to prepare the nanofluid following the two-step method. The thermal conductivity coefficient of the nanofluid was measured using the KD2-Pro thermal analyzer. Findings showed mass fractions of Er_2O_3 and Co_3O_4 nanoparticles, and temperatures affected the thermal conductivity. Results showed that the Er_2O_3/EG and Co_3O_4/EG nanofluid recorded higher thermal conductivity than the base fluid. Results also showed the nanofluid thermal conductivity increased by almost 2.26% and 5.38% at 20 °C and 50 °C, respectively, at 0.5 vol%. Measurements found that the maximum thermal conductivity of 6.85% prevailed at 50 °C in the volume fraction of 0.5 vol %. The obtained thermal conductivity results in the present experimental of Co_3O_4 nanofluid are compared with previous literature study results. Finally, these results are promising about using Er_2O_3/EG and Co_3O_4 /EG nanofluid in a solar thermal application.

References

[1] Alsboul, Monther, Mohd Sabri Mohd Ghazali, Mohamed R. Gomaa, and Aliashim Albani, Nanomaterials **12**, 2779 (2022).
[2] Alsboul, Monther, Mohd Sabri Mohd Ghazali, Mohamed R. Gomaa, and Aliashim Albani, Chemical Engineering & Technology **45**, 2139-2149 (2022).
[3] Behera, U.S., Sangwai, J.S. and Byun, H.S. Renewable and Sustainable Energy Reviews, **207**, 114901 (2025).
[4] Zou, Quanle, Tengfei Ma, Jinyan Liang, Bochao Xu, and Qican Ran. International Journal of Rock Mechanics and Mining Sciences **188**, 106056 (2025).

O36. Development and Characterization of PEG-CMC-CNT Containing Hydrogels for Drug Delivery Systems

Dilek BAYRAKDAR[1*], Mohmad ABOBAKER[1], Serbülent TÜRK[2], Burak ÜNLÜ[2] , Mediha İpek[1,3]

[1]Biomedical Engineering, Institute of Natural Sciences, Sakarya University, Esentepe Campus, 54187 Sakarya, Türkiye https://ror.org/04ttnw109

[2]Biomedical, Magnetic and Semi Conductive Materials Research Center (BIMAS-RC), Sakarya University, Esentepe Campus, 54187 Sakarya, Türkiye https://ror.org/04ttnw109

[3]Department of Metallurgy and Materials Engineering, Faculty of Engineering, Sakarya University, Esentepe Campus, 54187 Sakarya, Türkiye https://ror.org/04ttnw109

**+90 552 260 2928, dilek.bayrakdar@ogr.sakarya.edu.tr*

Hydrogels are flexible and soft polymeric network structures that can retain high amounts of water in their structure and are biocompatible. Compared to traditional drug delivery methods, hydrogels enable controlled drug release in the targeted area and prevent unwanted side effects. Additionally, hydrogels have a significant drug loading capacity due to their porous structure and are easily excreted from the body due to their biodegradable properties[1]. It is very important to design and develop new drug delivery systems to reduce the side effects of drugs such as DOX used to treat cancer, maximize their effectiveness, and improve patient-drug compliance[2]. In this study, PEG, CMC, and CNT components were combined at different concentrations for use in drug delivery systems, and hybrid hydrogels were synthesized using physical mixing and cross-linking techniques[3]. PEG is a polymer that is non-toxic, water-soluble, and quickly eliminable from the body[4]. The CMC component has properties such as biocompatibility, biodegradability, and low cost. In drug delivery systems, CMC causes slow release, maintaining the drug concentration at a controlled level for an extended period. This minimizes drug side effects[5]. CNT hydrogel drug delivery systems exhibit unique optical, physical, and electrical properties compared to traditional hydrogels[6]. In the synthesized hydrogels, PEG and CMC impart biocompatibility and biodegradability properties to the system, while the CNT component increases the loading capacity of chemotherapy drugs due to its large surface area[4], [5], [6].

Characterization studies were conducted to evaluate the structure and properties of the synthesized hydrogels: FTIR analysis was performed to investigate the chemical interactions between PEG, CMC polymers, and CNT nanomaterials. XRD analysis was performed to investigate the crystal structure of PEG-CMC-CNT hydrogels. The surface charge and potential stability of the synthesized hydrogels were examined by measuring the zeta potential, while the size distribution of the hydrogel particles was examined by measuring the particle size [3]. As a result of zeta potential measurements, S1 (%4PEG20000-%2CMC-%0.5CNT), S2 (%10PEG20000-%2CMC-%0.5CNT), S3 (%10 PEG8000, %2 CMC, %0.5 CNT), and S4 (%10 PEG8000, %2 CMC, %1 CNT) samples reported values of 1.12 mV, -51.04 mV, -31.48 mV, and -0.5 mV, respectively. The zeta potential measurement values of the other components used in the synthesis were recorded as follows: PEG20000: -2.62 mV, PEG8000: -0.83 mV, CMC: -0.01 mV, CNT: -8.45 mV, TX-100: 0.97 mV, and GA: -15.59 mV. Figure 1 shows the zeta potential measurement graph prepared with the zeta potential measurements of the hydrogel samples synthesized and the other components used in the synthesis (PEG20000, PEG8000, CMC, CNT, TX-100, GA). Zeta potential analysis revealed that hydrogel systems containing CNTs and PEG20000 exhibited high electrostatic stability. The zeta value became more negative in systems cross-linked with glutaraldehyde, while it was closer to zero in systems containing only PEG or CMC.

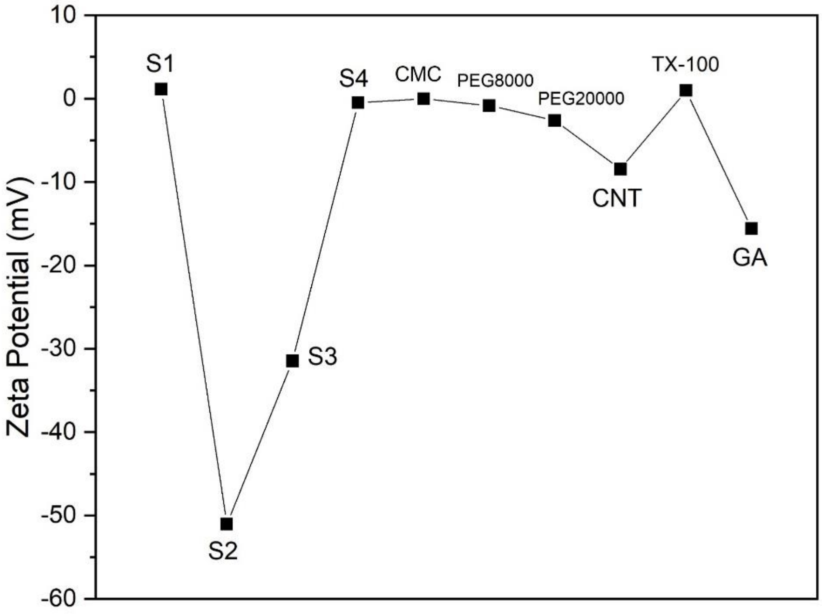


Fig. 3. Zeta potential measurement

In general, PEG and CMC give biocompatibility and degradability to drug delivery systems, while CNTs increase mechanical strength and potential drug loading capacity. This study focuses on the synthesis and characterization of PEG-CMC-CNT hydrogels with the aim of developing innovative targeted drug delivery systems and new strategies for cancer treatment.

Acknowledgement

This work was supported by the Scientific Research Projects Commission of Sakarya University (Project Number: 2025-27-70-27).

References

[1] P. Kesharwani, A. Bisht, A. Alexander, V. Dave, and S. Sharma, “Biomedical applications of hydrogels in drug delivery system: An update,” *J. Drug Deliv. Sci. Technol.*, vol. 66, no. June, p. 102914, 2021, doi: 10.1016/j.jddst.2021.102914.

[2] A. Ansary, A. Osman, and M. E. El-Khouly, “Doxorubicin-loaded pH-responsive porphyrin-derived carbon dots as a promising biocompatible drug delivery system for effective chemotherapy of breast cancer,” *RSC Adv.*, vol. 15, no. 9, pp. 6457–6473, 2025, doi: 10.1039/d4ra09058f.

[3] M. H. Alizadeh, M. Pooresmaeil, and H. Namazi, “Carboxymethyl cellulose@multi wall carbon nanotubes functionalized with Ugi reaction as a new curcumin carrier,” *Int. J. Biol. Macromol.*, vol. 234, no. February, p. 123778, 2023, doi: 10.1016/j.ijbiomac.2023.123778.

[4] M. Vashist, Arti , Kaushik, Ajeet , Vashist, Atul, Sagar, Vidya , Ghosal, Anujit, Gupta, Y. K., Ahmad, Sharif and Nair, “Advances in Carbon Nanotubes Hydrogel Hybrids in Nanomedicine for Therapeutics.pdf.”

[5] N. F. C. Nan, N. Zainuddin, and M. Ahmad, “Preparation and swelling study of CMC hydrogel as potential superabsorbent,” *Pertanika Journal of Science and Technology*, vol. 27, no. 1. pp. 489–498, 2019.

[6] G. Cirillo, S. Hampel, U. G. Spizzirri, O. I. Parisi, N. Picci, and F. Iemma, “Carbon nanotubes hybrid hydrogels in drug delivery: A perspective review,” *Biomed Res. Int.*, vol. 2014, 2014, doi: 10.1155/2014/825017.

O37. Preparation and Characterization of Smart Hydrogel Drug Delivery System

Mohmad ABOBAKER[1*], Dilek BAYRAKDAR[1], Serbülent TÜRK[2], Burak ÜNLÜ[2]
[1]*Biomedical Engineering, Institute of Natural Sciences, Sakarya University, Esentepe Campus, 54187 Sakarya, Türkiye* https://ror.org/04ttnw109
[2]*Biomedical, Magnetic and Semi Conductive Materials Research Center (BIMAS-RC), Sakarya University, Esentepe Campus, 54187 Sakarya, Türkiye* https://ror.org/04ttnw109
**+90 535 784 6537, mohmad.abobaker1@ogr.sakarya.edu.tr*

Hydrogels are biomaterials with unique properties and three-dimensional polymeric network structure produced for use in various applications in the biomedical area [1]. Hydrogels are similar to living tissues as they are structures with high water content. Different properties of polymers are utilized to synthesize new hydrogels [2]. By evaluating issues such as drug release behavior, biocompatibility, and optimization of mechanical and chemical properties of the new hydrogels obtained, an innovative material contribution to literature can be provided.

Smart hydrogels exhibit swelling and degradation behavior depending on the chemical structure and cross-link density of polymers under the influence of environmental conditions or enzymes in the biological environment [1]. In drug delivery system applications, the degradation of smart hydrogels after a certain period of time enables the drug to be released at the desired location. Thus, the drug loaded into the drug delivery system (DOX, etc.) can be released in the appropriate environment and location[3]. Controlled release systems, which is one of the most important smart hydrogels, have become an important material that can increase patient comfort due to their features such as being developable, biocompatible, sustainable, economical and reliable [4]. DOX is a potent anti-cancer drug used in cancer treatment [5]. Controlled release systems are needed to reduce the unwanted side effects of the drug which is at the drug delivery system.

In this study, a biocompatible hydrogel drug delivery system was designed using a combination of chitosan-sodium alginate-Pluronic 123 (CS/SA/P123) polymers to provide the controlled release of the drug DOX. The synthesized hydrogel drug delivery system has the potential for controlled drug release thanks to its pH and temperature sensitivity. The CS/SA/P123 hydrogels were prepared using a physical mixing method.

Particle size and zeta potential measurements were performed using Dynamic Light Scattering (DLS). The particle sizes of the synthesized hydrogels were found to be 1067 nm for H1 (5% P123-1% CH-2% SA) and 1196.9 nm for H2 (10% P123-1% CH-2% SA). P123 alone formed nanostructures with dimensions of 276.5 nm. CH and SA formed large aggregates with dimensions of 2353.5 nm and 1983.4 nm, respectively. Figure 1 shows the cumulative particle size measurements for all polymers used and the synthesized hydrogels. By zeta potential analysis, sample H2 exhibited high colloidal stability with a value of -59.36 mV, while sample H1 remained within acceptable limits around -29.38. P123, CH, and SA, respectively; It showed values of -49.34 mV, -10.29 mV, and -61.07. Figure 2 shows the zeta potential measurement graphs created with these values.

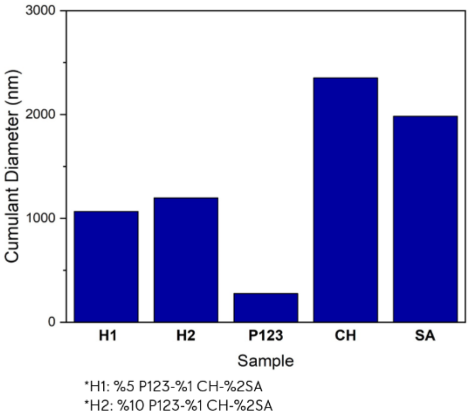


Fig. 1. Cumulative particle sizes

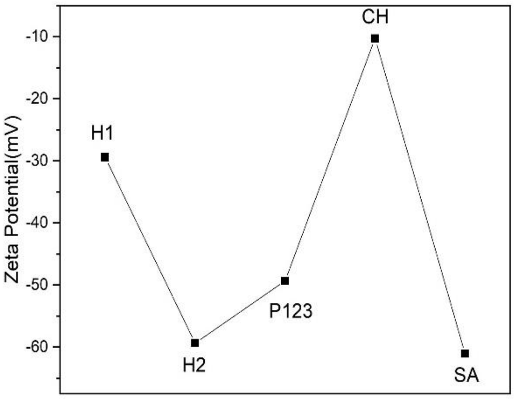


Fig. 2. Zeta potential measurement

Chemical characterization of the structures was performed using Fourier Transform Infrared Spectroscopy (FTIR). Figure 3 shows the FTIR analysis graphs of the H1 and H2 hydrogels. In sample H1, –OH and –NH_2 vibrational bands in the range of 3200–3600 cm^{-1}, as well as bands at 1650 cm^{-1} (C=O) and 1050–1150 cm^{-1} (C–O), confirmed the presence of biopolymers. Sample H2 exhibited weaker spectral signals reflecting the dominant chemical structure of P123. These findings demonstrate the potential suitability of the CS/SA/P123 hydrogel system for structural stability, particle size control, and smart drug delivery applications.

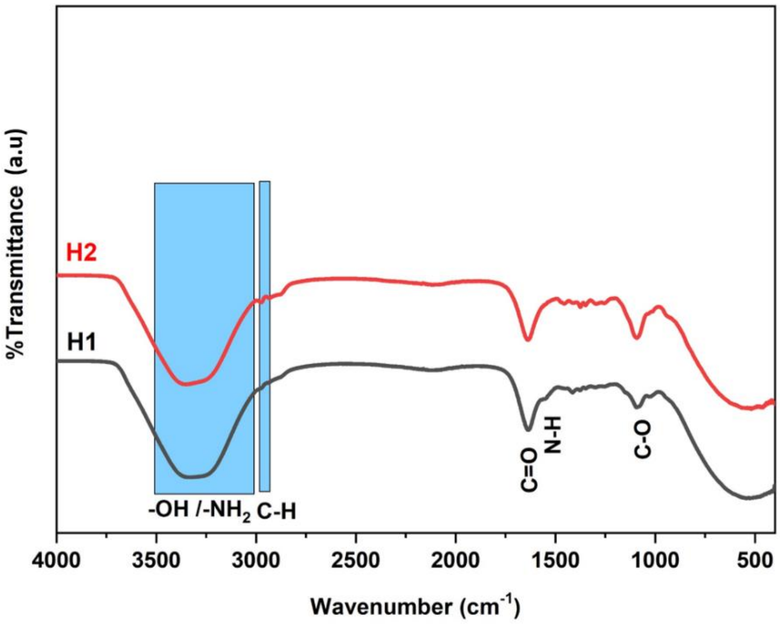


Fig. 3. FTIR analysis of synthesized hydrogels

References

[1] A. Bordbar-Khiabani and M. Gasik, “Smart Hydrogels for Advanced Drug Delivery Systems,” *International Journal of Molecular Sciences*, vol. 23, no. 7. 2022. doi: 10.3390/ijms23073665.

[2] P. Kesharwani, A. Bisht, A. Alexander, V. Dave, and S. Sharma, “Biomedical applications of hydrogels in drug delivery system: An update,” *J. Drug Deliv. Sci. Technol.*, vol. 66, no. June, p. 102914, 2021, doi: 10.1016/j.jddst.2021.102914.

[3] K. S. Soppimath, T. M. Aminabhavi, A. M. Dave, S. G. Kumbar, and W. E. Rudzinski, “Stimulus-responsive ‘smart’ hydrogels as novel drug delivery systems,” *Drug Dev. Ind. Pharm.*, vol. 28, no. 8, pp. 957–974, 2002, doi: 10.1081/DDC-120006428.

[4] N. Kumar, B. Ghosh, A. Kumar, R. Koley, S. Dhara, and S. Chattopadhyay, “Multilayered ‘SMART’ hydrogel systems for on-site drug delivery applications,” *J. Drug Deliv. Sci. Technol.*, vol. 80, no. July 2022, p. 104111, 2023, doi: 10.1016/j.jddst.2022.104111.

[5] C. Carvalho *et al.*, “Doxorubicin: The Good, the Bad and the Ugly Effect.” Current Medicinal Chemistry, pp. 3267–3285, 2009.

O38. Nanotechnology and nanocarrier vaccine in aquaculture

Erlong Wang (welsicau@126.com)
College of Animal Science and Technology, Northwest A&F University, Yangling, Shaanxi 712100, China

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

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

Poster presentations

P1. Zn-MOF as an efficient catalytic platform for the conversion of waste polyethylene terephthalate bottles into bis(2-hydroxyethyl) terephthalate

Rubi Bhakhar[1] Rik Rani Koner[2*]
[1]School of Chemical Sciences and Advanced Materials Research Center, Indian Institute of Technology Mandi, Kamand, Mandi 175075, Himachal Pradesh, India.
[2]School of Mechanical and Materials Engineering, Indian Institute of Technology Mandi, Kamand, Mandi 175075, Himachal Pradesh, India.
**Corresponding author: rik@iitmandi.ac.in*
Presenter's Address - +918708879230, d22066@students.iitmandi.ac.in

Non-biodegradable plastics, such as polyethylene terephthalate (PET), are common ingredients utilized in packaging materials and pose numerous threats worldwide due to their lack of biodegradability. Non-degradability and recycling issues have made PET a major environmental challenge. Several strategies and materials have been employed to convert PET into value-added chemicals, including bis(2-hydroxyethyl) terephthalate (BHET). Glycolysis of PET is one of the common approaches to convert the plastic, PET into BHET. Metal-organic frameworks (MOFs) have been employed as catalysts for the conversion of PET into BHET. Herein, we have developed a Zn-based MOF through a solvothermal mixed-ligand strategy from the reaction of Zn (II), 2,6-naphthalene dicarboxylic acid, and 2,2 bipyridine. This Zn-MOF displayed remarkable catalytic activity for the conversion of PET into BHET through glycolysis. The reaction parameters, such as reaction time, reaction temperature, catalyst loading, and amount of ethylene glycol, were optimized to understand the best operating conditions of the Zn-MOF. Zn-MOF achieved 100% conversion of PET, giving a BHET yield of 82.8% at 180 ℃ within 7 h.

References

[1] Yang R-X, Bieh Y-T, Chen CH, Hsu C-Y, Kato Y, Yamamoto H, et al. ACS Sustainable Chemistry & Engineering., **9**, 6541-50 (2021).
[2] Wu Y, Wang X, Kirlikovali KO, Gong X, Atilgan A, Ma K, et al. Angew. Chem. 2022, **61**, 202117528 (2022).

P2. Anelastic-elastic body of nanocomposites of multiwalled carbon nanotubes and polymers, SiO_2

A.P. Onanko[*], M.V. Yatsiuk, Y.A. Onanko, O.P. Dmytrenko, M.P. Kulish, T.M. Pinchuk-Rugal, D.V. Charnyi, E.M. Matselyuk, O.L. Pavlenko, T.O. Busko, A.M. Gaponov, O.G. Rugal, L.I. Kurochka, P.P. Ilyin, S.V. Marysyk
[*]*Kyiv national university, Kyiv, Ukraine, onanko@i.ua*

Abstract

Anelastic, elastic characteristics, anelastic-elastic body of radiation and structural functionalized nanocomposites of polyamide, polyethylene, polyvinylchloride, SiO_2 and multiwalled carbon nanotubes (MWCNT) is represented.

Introduction

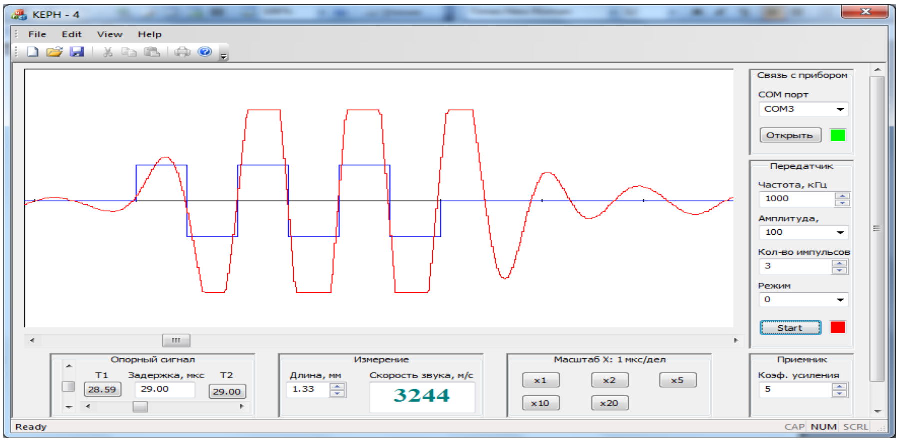
Mechanical characteristics of nanocomposites based on polyamide, polyethylene, polyvinylchloride with MWCNT, in which atoms number on the surface is compared to the total atoms number, the dimensions of which at least in one direction, range from several to hundreds nm, fundamentally differ from mechanical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

Experimental Methods

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

Results and Discussion

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



Связь с прибором
COM порт: COM3

Передатчик
Частота, кГц: 1000
Амплитуда,: 100
Кол-во импульсов: 3
Режим: 0

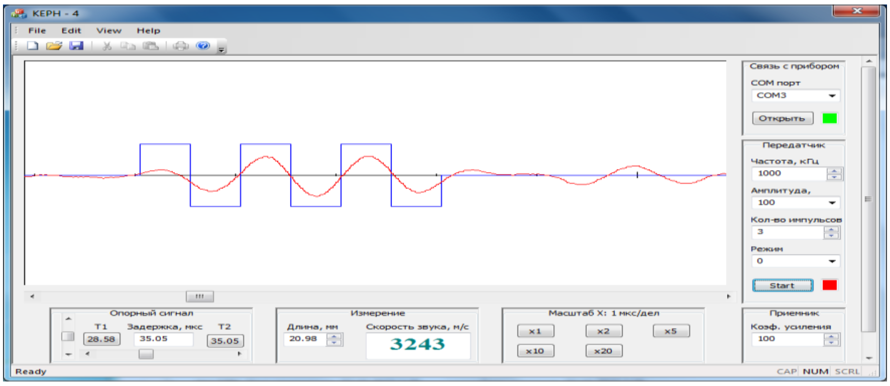
Опорный сигнал
T1: 28.59
Задержка, мкс: 29.00
T2: 29.00

Измерение
Длина, мм: 1.33
Скорость звука, м/с: 3244

Масштаб X: 1 мкс/дел

Приемник
Коэф. усиления: 5

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



Связь с прибором
COM порт: COM3
Передатчик
Частота, кГц: 1000
Амплитуда,: 100
Кол-во импульсов: 3
Режим: 0
Опорный сигнал
T1: 28.58
Задержка, мкс: 35.05
T2: 35.05
Измерение
Длина, мм: 20.98
Скорость звука, м/с: 3243
Масштаб X: 1 мкс/дел
Приемник
Коэф. усиления: 100

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

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

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

$$\mu = -\frac{\varepsilon_\perp}{\varepsilon_\parallel} = \frac{\frac{1}{2}V_\parallel^2 - V_\perp^2}{V_\parallel^2 - V_\perp^2} = ½\left[1 + \frac{1}{1-\left(\frac{V_\parallel}{V_\perp}\right)^2}\right]. \tag{2}$$

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

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

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

Complex elastic modulus of nanocomposite polyamide-6 (PA-6) $(NH(CH_2)_5CO)_n$ + % MWCNT E* is equal to the sum of elastic dynamic modulus $E' = \rho V_\parallel^2$ and loss modulus $E'' = E'\delta$ [3]:

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

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

$$\frac{E''}{E'} = \delta = \pi Q^{-1} = \propto \lambda = \propto \frac{V}{f}, \tag{5}$$

where α - US attenuation coefficient, λ - US wavelength, f - US frequency. IF is equal $Q^{-1} = \delta/\pi$. The logarithmic decrement of attenuation δ of US oscillations with amplitude $A = A_0e^{-\delta x}$ is equal:

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

Conclusions

1. The presence of the strong interaction for nanocomposite between polyamide-6 $(NH(CH_2)_5CO)_n$ and multiwalled carbon nanotubes was confirmed.

2. The increase of the nanocomposite crystallinity degree at growth of multiwalled carbon nanotubes concentration filling with the nanotubes of matrix results in the decline of content of organized phase.

3. The phenomenon of change of Poisson coefficient μ, Debye temperature θ_D, dynamic elastic modulus $E' = \rho V_{\parallel}^2$, dynamic shear modulus $G = \rho V_{\perp}^2$ under the influence of electronic e^- radiation is caused by the appearance of primary radiation defects (RD). As the result of interdefect interactions primary RD form secondary RD.

Acknowledgements

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.

References

[1] Y.A. Onanko, L.V. Kuzmych, A.P. Onanko et al. *ECS Journal of Solid State Science and Technology,* **V. 13, № 4**, 045001(6) (2024).
DOI: https://iopscience.iop.org/article/10.1149/2162-8777/ad36e0

[2] A.P. Onanko, L.V. Kuzmych, Y.A. Onanko et al. *J. Materials Research Express,* **V. 10 № 10**, 106511(7) (2023)
DOI: https://iopscience.iop.org/article/10.1088/2053-1591/acfecc

[3] A.P. Onanko, V.V. Kuryliuk, Y.A. Onanko et al., *J. Nano-Electron. Phys.*, **V. 14, № 6**, 06029(7) (2022).
DOI: https://doi.org/10.21272/jnep.14(6).06029.

[4] A.P. Onanko, V.V. Kuryliuk, Y.A. Onanko et al., *J. Nano-Electron. Phys.*, **V. 13, № 5**, 05017(5) (2021).
DOI: https://doi.org/10.21272/jnep.13(5).05017.

[5] A.P. Onanko, V.V. Kuryliuk, Y.A. Onanko et al., *J. Nano-Electron. Phys.*, **V. 12, № 4**, 04026(5) (2020).
DOI: https://doi.org/10.21272/jnep.12(4).04026

P3. Optoelectronic and magnetic properties of RE= Sm, Eu, Gd, and Er doped zinc sulphide

H. HEDJAR[1, 2, *], S.DERKAOUI[2], A.H.TABTI[2], A.BOUKORTT[1].
[1]Elaboration and Characterization Physico-Mechanical and Metallurgical of Materials Laboratory (ECP3M), Abdelhamid Ibn Badis University-Mostaganem. Route Nationale N◦11, Kharrouba, 27000, Mostaganem, Algeria
[2]Tissemsilt University, Algeria
[*] +213697060006
H.hedjar@univ-tissemsilt.dz
Hakima13kima@gmail.com

We present a theoretical study of the electronic structure, magnetic and optical properties of RE-doped zinc sulphide (RE = Sm, Eu, Gd, and Er) in a zinc blende phase, which is investigated using the spin-polarized spin density functional theory (spin-DFT). The First-principles calculations based on density functional theory and the full-potential linearized augmented plane wave method (FP-LAPW) are performed by employing the GGA + U (U is the Hubbard term of the Coulomb repulsion correlation) approximation. The lattice parameter will increase by RE doping ZnS. The total density of states (TDOS) and partial density of states (PDOS) show that all the systems have half-metallic character behaviour with 100% spin polarization at the Fermi level provided by the RE-4f states except ZnS: Eu it has a semiconductor character. The values of differences in total energy ΔE indicate that ZnS: Sm, ZnS: Eu, and ZnS: Er are stable in the ferromagnetic phase. However, ZnS: Gd favours the AFM phase. The total magnetic moment of all systems is very interesting. All systems showed significant redshift except ZnS: Eu, and all exhibited broad absorption in the UV region. Doping by RE is a feasible method to enhance the electronic, magnetic, and optical properties of ZnS for the new generation of optoelectronic and spintronic applications.

References

[1] D.E. Aimouch, S. Meskine, A. Boukortt, A. Zaoui, J. Magn. Magn Mater. 451 (2018) 70–78.
[2] J.K. Furdyna, J. Kossut 25, Academic Press, New York, 1988.
[3] H. Ohno, Science 281 (1998) 951.
[4] J. Blinowski, P. Kacman, J.A. Majewski, Phys. Rev. B 53 (1996) 9524.

P4. Synthesis, Characterization, and Antimicrobial Evaluation of SiO_2/5-ASA and SiO_2/5-ASA/Ag Nanomaterials

Miljana M. Dukić*, Katarina Isaković, Valentina Nikšić, Dušan N. Sredojević, Vesna M. Lazić

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

**miljana.dukic@vin.bg.ac.rs, +381616179137*

This study reports on the synthesis, characterization, and antimicrobial evaluation of two types of nanomaterials. The first nanomaterial involves surface-modified SiO_2 nanoparticles functionalized with 5-aminosalicylic acid (5-ASA), forming an organic-inorganic hybrid nanomaterial. SiO_2/5-ASA. The second structure includes the incorporation of silver nanoparticles (Ag NPs) into the SiO_2/5-ASA structure, resulting in the SiO_2/5-ASA/Ag nanocomposite. The study focuses on understanding these nanomaterials' structural and electronic properties, employing various characterization techniques such as Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), and UV-Vis spectroscopy. These experimental techniques were bolstered by density functional theory (DFT) calculations to provide deeper insights into the materials' behaviors at the atomic and molecular levels. The experimental UV-Vis and FTIR spectra align with the theoretical results obtained through DFT, confirming the accuracy of the chosen computational models. Preliminary XRD analysis confirmed the successful incorporation of Ag nanoparticles into the SiO_2/5-ASA matrix, suggesting that the Ag NPs were well-distributed within the hybrid structure. However, further details on the morphology and distribution of the Ag NPs within the nanomaterial are being analyzed using transmission electron microscopy (TEM), The antimicrobial activity of the synthesized materials was assessed against three pathogenic microorganisms: Gram-negative bacteria *Escherichia coli*, Gram-positive bacteria *Staphylococcus aureus* and fungus *Candida albicans*. The results indicated that SiO_2/5-ASA exhibited enhanced antimicrobial efficacy compared to the SiO_2/5-ASA/Ag composite, as this performance was primarily attributed to the presence of the free NH_2 group in 5-ASA. The findings of this research highlight the multifunctional potential of organically modified SiO_2 nanomaterials in antimicrobial applications, demonstrating their capability to serve as effective antimicrobial agents while being supported by both experimental and theoretical analyses. The promising results open avenues for further exploration of these materials in various biomedical and environmental applications, where antimicrobial properties are important.

P5. 3D statistical tolerance synthesis in mechanical assemblies

Said Boutahari *, Mustapha El Mouden, Mouhssine Chahbouni
TSI laboratory, Higher school of technology, Sidi Mohammed Ben Abdellah University
Imouzzer street, BP 2626 (30000), Fez, Morocco
**+212 6 60 41 73 67, said.boutahari@usmba.ac.ma*

Cost and manufacturing accuracy are closely related in many industries. The cost and quality of products are significantly impacted by the tolerances chosen. 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. Therefore, one of the most crucial steps in design optimization is choosing tolerances.

Based on the Jacobian torsor model, this study suggests a statistical method for redefining geometric tolerances.

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. Statistical limits are then found using Monte Carlo simulation. 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 real-world case study is used to demonstrate the efficacy of the suggested method.

P6. Development and characterization of honokiol-loaded liposomes

Karolina Olechowska [*]
Department of Environmental Chemistry, Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387, Kraków, Poland
[*] *0048 12 686 25 68, karolina.weder@uj.edu.pl*

Antimicrobial agents play a crucial role in the treatment of bacterial infections. However, their excessive use over the past decades has resulted in a dramatic increase in antimicrobial resistance, which is now considered one of the greatest threats to global public health in the 21st century[1]. The urgent demand for novel, effective and safe antimicrobial substances and increasing environmental awareness has led to an intensified search for antimicrobials of a natural origin.

Honokiol (5,3'-diallyl-2,4'-dihydroxydiphenyl) is a neolignan derived from *Magnolia* species. It exhibits a broad spectrum of pharmacological properties, including anticancer, anti-inflammatory, antioxidant, and neuroprotective effects[2]. What is more, honokiol has demonstrated significant antibacterial activity against various Gram-positive and Gram-negative pathogens, making it a promising candidate for antimicrobial applications[3]. However its therapeutic potential is limited because of the low water solubility. To overcome this problem, the development of appropriate delivery systems seems to be crucial. In recent years, nanotechnology-based honokiol delivery systems have gained extensive attention for their promising applications in medicine[4]. However to date, there are no works investigating honokiol delivery systems in the context of its antibacterial properties.

The aim of the presented work was to develop and optimize honokiol-loaded liposomal delivery system to enhance the antibacterial efficacy of honokiol. The investigations were performed for liposomes composed of phosphatidylcholine, cationic lipid DOTAP, β-sitosterol (a plant sterol with antibacterial properties) or cholesterol, and honokiol. To achieve optimal encapsulation efficiency and stability, different lipid compositions, honokiol-to-lipid ratios, total lipid concentrations and preparation conditions were tested. The properties of the formulations containing either cholesterol or β-sitosterol were evaluated as a preliminary step toward verifying the potential synergistic effects of honokiol and β-sitosterol.

Acknowledgments

This work has been supported by a grant from the Faculty of Chemistry under the Strategic Program Excellence Initiative at Jagiellonian University.

References

[1] https://www.who.int/docs/default-source/antimicrobial-resistance/amr-factsheet.pdf
[2] A. Rauf et al, *Phytomedicine*, **90**, 153647 (2021).
[3] K. Chiu, *J Formos Med Assoc*, **120**, 827 (2021).
[4] J. Yang et al, *Int J Nanomedicine*, **18**, 6639 (2023).

P7. Development of new type core-shell thermochromic pigments based on selected triarylmethane dyes

Bartosz Kopyciński[1,2*], Alicja Duda[3], Sebastian Jurczyk[1],
Grażyna Kamińska-Bach[1], Małgorzata Zubielewicz[1], Katarzyna Jaszcz[4]
[1] *Łukasiewicz Research Network – Institute for Engineering of Polymer Materials and Dyes,*
M. Skłodowskiej-Curie 55 St., 87-100 Toruń, Poland
[2]*Doctoral School, Silesian University of Technology,*
Akademicka 2A St., 44-100 Gliwice, Poland
[3]*Łukasiewicz Research Network – Institute of Non-Ferrous Metals,*
gen. J. Sowińskiego 5 St., 44-100 Gliwice, Poland
[4]*Department of Physical Chemistry and Technology of Polymers, Silesian University of Technology,*
ks. M. Strzody 9 St.,44-100 Gliwice, Poland
[*]*e-mail: bartosz.kopycinski@impib.lukasiewicz.gov.pl, tel. +48 32 231 90 41*

Thermochromic pigments exhibit the ability to change color in response to temperature changes. After absorbing a certain amount of heat, their crystalline or molecular structure undergoes a reversible change in such a way that it absorbs and emits light of a different wavelength than the initial state [1,2]. A method for the synthesis of new type core-shell thermochromic pigments based on selected triarylmethane dyes was proposed. Thus, a set of aqueous solutions of appropriate organic dyes in the form of sodium salts of various concentrations, which were protonated as needed, was subjected to colorimetric analysis. The selected solutions were emulsified using ecological, non-toxic surfactants used in the cosmetics and food sectors. Liquid, non-ionic emulsifiers with a hydrophilic-lipophilic balance index of 3÷6 were tested, enabling the production of water-in-oil emulsions. The next step was to encapsulate the obtained emulsions. A self-organizing organosilicon polymer, undergoing hydrolytic cross-linking at the polymer-water interface, was chosen as the matrix material of the capsules. The separated product consisted of pigments in the form of capsules with polymer shells, which were characterized using selected spectroscopic, thermal and microscopic methods. The following hypotheses were confirmed. The first one, that there are organic dyes whose aqueous solutions at a specific concentration and pH value exhibit a reversible color change $\Delta E \geq 5$ depending on the ambient temperature, i.e. at 20 or -18°C. And the second one, that by encapsulating emulsified aqueous solutions of selected organic dyes in a polymer matrix, it is possible to synthesize pigments capable of reversible color change $\Delta E \geq 5$ depending on the ambient temperature, i.e. at 20 or -80°C (Fig. 1). In summary, the procedure described above allows for the synthesis of stable, mostly reversible thermochromic pigments with micrometric dimensions ($d_{50}<10$ μm) which can be used as indicators for monitoring the state of deep freezing. The obtained pigments will be applied at further stages of research as components of functional thermochromic coatings for covering various types of substrates.

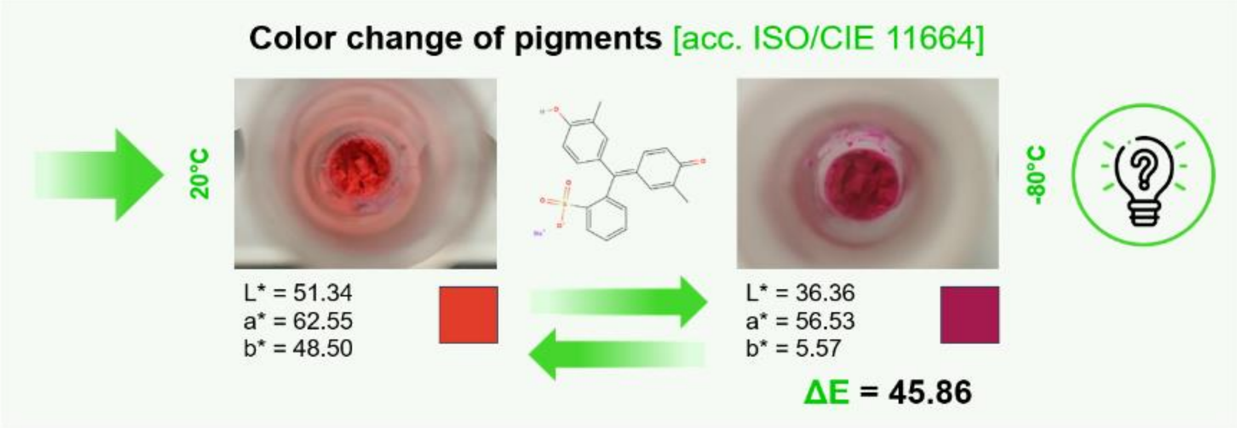


Figure 4. Color-temperature correlation for one of the developed pigments

Acknowledgments

This work was financially supported by the Polish Ministry of Education and Science as part of the Implementation Doctorate Program (Grant no. RJO15/SDW/006-16).

References

[1] B. Kopyciński, A. Duda, M. Zubielewicz, and K. Jaszcz, *Ochrona przed Korozją*, **67(6)**, 152-164 (2024).

[2] B. Liu, A. R. Mazo, P. A. Gurr, and G. G. Qiao, *ACS Applied Materials & Interfaces Journal*, **12**, 9782-9789 (2020).

P8. Water-based organic coatings with bioactive and camouflage properties for the protection of military equipment

Bartosz Kopyciński[1,2], **Ewa Langer[1*]**, Maja A. Zaczek-Moczydłowska[3],
Andrzej Hudecki[4], Alicja Hryniszyn[4], Mariola Bodzek-Kochel[1], Marek Łos[3]
[1] Łukasiewicz Research Network – Institute for Engineering of Polymer Materials and Dyes,
M. Skłodowskiej-Curie 55 St., 87-100 Toruń, Poland
[2]Doctoral School, Silesian University of Technology,
Akademicka 2A St., 44-100 Gliwice, Poland
[3]Biotechnology Centre, Silesian University of Technology,
B. Krzywoustego 8 St., 44-100 Gliwice, Poland
[4] Łukasiewicz Research Network – Institute of Non-Ferrous Metals,
gen. J. Sowińskiego 5 St., 44-100 Gliwice, Poland
[*]e-mail: ewa.langer@impib.lukasiewicz.gov.pl, tel. +48 32 231 90 41

Camouflage coatings are a special case of organic functional coatings. Masking paints are intended for camouflage painting of military equipment. Camouflage painting made with a set of paints with specific spectral characteristics ensures the appropriate degree of tools and machines camouflage used by the armed forces [1,2]. Water-based paints for masking covering of protective masks printed using selective laser sintering technology from thermoplastic polyurethane in green, brown, and black colours have been developed. The functionality of such coatings was additionally increased by giving them bioactive properties, which was achieved by enriching the camouflage paint formulas with the addition of silver-based compounds. The following bioactive components were used: nanosilver on colloidal silica, silver sodium hydrogen zirconium phosphate, and self-synthesized silver powder in an amount of 0.625, 1.25, 2.5 or 5 wt%. The paints' application potential was defined, among others, by determining the re-emission coefficient and testing the resistance to delamination from the substrates as a result of cutting the coating. The developed coatings were also tested for antiviral activity using a neutral-red-based cytopathic effect assay, which was analyzed using a smartphone. The antiviral activity was assessed in triplicates using the reference human coronavirus 229E and the human fibroblast cell line MRC-5. It has been shown that, thanks to the use of appropriate pigments, discussed paints meet the camouflage requirements (Fig. 1) specified by the Polish military standard [3] and are characterized by excellent adhesion to thermoplastic polyurethane. Moreover, the cytopathic effect assay that was performed indicated efficient antiviral activity of coatings consisting of nanosilver on colloidal silica and silver sodium hydrogen zirconium phosphate, as assessed by a reduction of viral infectivity in comparison to negative and positive controls and microscopic evaluation. Due to the above, the correct formulation of liquid paints, including the selection of a polymer binder, pigments, auxiliaries and bioactive compounds, made it possible to obtain coloured, functional coatings that can be applied in the defense industry.

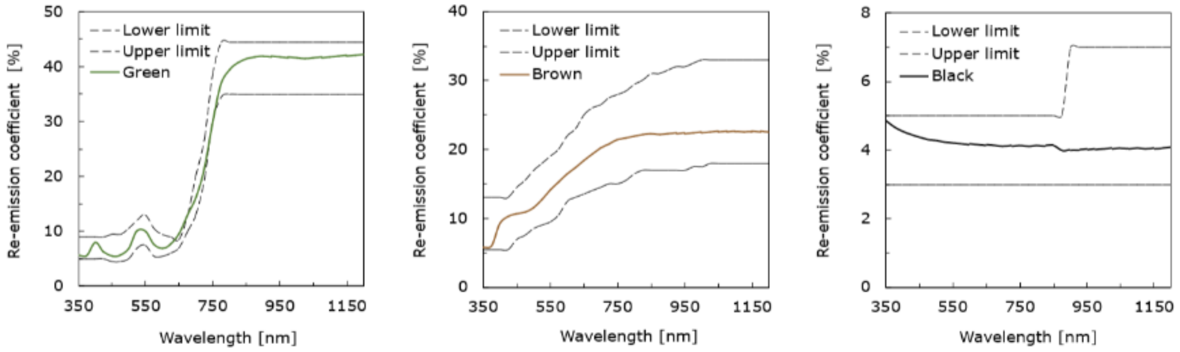


Figure 5. Re-emission coefficient of developed paints (camouflaging ability)

Acknowledgments

This work was financially supported by the National Centre for Research and Development (Grant no. DOB-SZAFIR/02/B/004/02/2021).

References

[1] F. Xue, S. Xu, Y-T. Luo, and W. Jia, *Neurocomputing*, **172(8)**, 262-270 (2014).
[2] Q. Jia, W. D. Xu, J. H. Hu, J. Liu, X. Yang, and L. Y. Zhu, *Multimedia Tools and Applications*, **79**, 22047-22064 (2020).
[3] NO-80-A200 Farby specjalne do malowania maskującego -- Wymagania i metody badań.

P9. PLGA-based nanoparticles for targeted drug delivery in Immuno-Oncology therapy

Inês S. Pinto[1,2,*], Annalee W. Nguyen[3], Jennifer A. Maynard[3], Henrique Faneca[2,4]

[1]University of Coimbra, Institute for Interdisciplinary Research, Doctoral Programme in Experimental Biology and Biomedicine (PDBEB), Portugal
[2]Center for Neuroscience and Cell Biology, University of Coimbra, 3004-504 Coimbra, Portugal
[3]Department of Chemical Engineering, University of Texas, Austin, TX 78712, USA
[4]Institute of Interdisciplinary Research (III), University of Coimbra, Casa Costa Alemão - Pólo II, 3030-789 Coimbra, Portugal
**inespinto@cnc.uc.pt*

The increasing incidence of cancer in population underscores the need for innovative therapeutic strategies that address the unique challenges posed by the tumour microenvironment and immune system alterations [1,2]. T-cell-based immunotherapies offer a promising approach due to their high specificity and antitumor activity. However, T-cell exhaustion and death remain major barriers as they facilitate immune evasion by tumors [3,4]. In this study, we present a nanosystem composed of poly(ethylene glycol)-block-poly(lactic acid-co-glycolic acid) (PEG-PLGA) nanoparticles designed to specifically deliver an immune checkpoint inhibitor (BMS-202) to T cells, enhancing their cytotoxic function. The nanoparticles feature a PLGA core that encapsulates the drug, while the PEG shell is functionalized with the F(ab')2 fragment of the CD3 antibody (Fab anti-CD3) to ensure targeted delivery to T cells. Our research explores the optimization of nanoparticle formulations, including polymer-to-drug molar ratios, physicochemical characterization, toxicity evaluation, and binding efficiency. We successfully optimized the formulation of PLGA-based nanoparticles to achieve a size below 200nm with a negative surface charge. Furthermore, the attachment of the Fab anti-CD3 was achieved using thiol-maleimide conjugation strategy, resulting in efficient antibody binding to the nanoparticles. Post-conjugation, the nanosystem showed an increase in particle size (from 165 nm to 182 nm) and a decrease in surface charge (from -20 mV to - 11mV), while maintaining stability with a low polydispersity index (<0.2). The optimized formulation exhibited an encapsulation efficiency of 33% and a drug loading capacity of 3.58 µg/mg polymer, with no observed cytotoxicity to T cells. Importantly, the nanosystem demonstrated specific targeting of T cells and efficient drug delivery, validating its potential as a targeted therapy for cancer patients. By enhancing the precision of T-cell immunotherapies, this work holds great promise for more effective cancer treatments. Ongoing optimizations aim to further enhance the therapeutic efficacy and clinical translation of this innovative strategy.

[1] B. Liu, H. Zhou, L. Tan, T. H. S. Kin, G. Xin-Yuan, *Sig Transduct Target Ther,* **9**, 175 (2024).
[2] L. Yutong, W. N. Annalee, A. M. Jennifer, *Curr Opin Biotechnol*, **78**, 102809 (2022).
[3] S.P. Inês, A. C. Rosemeyre, F. Henrique, *J Control Release*, **353**, 196–215 (2023).
[4] T. W. Garth, R. C. Marka, J. G. Michael, *Adv Radiat Oncol*, **3(4),** 520–526 (2018).

P10. Activated carbons from biomass for sustainable adsorption of emerging contaminants in water treatment

Tayra R. Brazil[1,2*], Valentina Silva[2], María V. Gil[3], Edson C. Botelho[1], Vânia Calisto[2]
[1] *Department of Materials and Technology, São Paulo State University, Guaratinguetá, Brazil.*
[2] *Department of Chemistry and CESAM, University of Aveiro, Aveiro, Portugal.*
[3] *Instituto de Ciencia y Tecnología del Carbono, INCAR-CSIC, Oviedo, Spain.*
**tayrabrazil@gmail.com*

Biomass represents a renewable, abundant, and carbon-neutral resource, whose importance has been growing due to pursuit a more sustainable industrial system. The occurrence and fate of pharmaceutical contaminants in aquatic environments constitute a critical issue, as these compounds can cause long-term damage to ecosystems and human health. Among them, antibiotics such as sulfamethoxazole (SMX) and trimethoprim (TMP), are of particular concern because they can promote bacterial resistance and are not fully removed by conventional wastewater treatment processes. In addition to antibiotics, psychoactive pharmaceuticals such as venlafaxine (VEN) are also considered contaminants of emerging concern. These issues highlight the urgent need for more effective and sustainable strategies to mitigate such emerging threats [1]. Adsorption using activated carbon (AC) has proven to be an effective technique for removing pharmaceutical contaminants from water, mainly due to the high specific surface area (S_{BET}) of these materials. The use of biomass as a precursor for AC contributes significantly to the sustainability of the process by avoiding non-renewable raw materials. In this context, ACs were produced from different biomass: coffee grounds (CG), Kraft lignin (KL), grape stems (GS), and olive pits (OP). Initially, biochars were obtained via conventional pyrolysis at 600 °C for 30 minutes under inert atmosphere. These biochars were then impregnated with KOH at a 1:1 mass ratio and subjected to microwave-assisted pyrolysis at 800 °C for 20 minutes, also under inert atmosphere. The resulting ACs were characterized by N_2 adsorption–desorption isotherms, revealing S_{BET} ranging from 345 to 1024 $m^2\,g^{-1}$ and total pore volumes between 0.17 and 0.47 $cm^3\,g^{-1}$. According to the International Union of Pure and Applied Chemistry (IUPAC) classification, the isotherms exhibited characteristics of both Type I and Type IV, indicating the coexistence of microporous and mesoporous structures. This hybrid pore structure suggests that the produced ACs have the potential to effectively adsorb a wide range of contaminants with varying molecular sizes. The produced materials were tested for the removal of three pharmaceutical contaminants: SMX, TMP, and VEN. The best performance was observed for the AC derived from coffee grounds, with adsorption percentage of 77, 64, and 44% for SMX, TMP, and VEN, respectively, highlighting that the nature of the precursor directly influences the properties of the ACs. Overall, the results obtained in this study demonstrate that the production of ACs from the evaluated biomass, using both conventional and microwave pyrolysis, is technically feasible. The resulting materials showed excellent surface area values and adsorption capacities, thus adding greater value to lignocellulosic residues that are abundant in the productive sector.

Acknowledgements

The authors acknowledge the financial support received from the Brazilian Funding Institution FAPESP (Fundação de Amparo à Pesquisa do Estado de São Paulo) (2023/07964-7) (2024/05202-5). The authors also acknowledge financial support to CESAM by FCT/MCTES (UIDP/50017/2020+UIDB/50017/2020+LA/P/0094/2020), through national funds. Valentina Silva support by Fundação para a Ciência e Tecnologia (FCT) PhD grant (2022.10472.BD).

References

[1] E. Menya, J. Jjagwe, H.M. Kalibbala, H. Storz, P.W. Olupot, Chemical Engineering Research and Design, **192**, 412-440.

P11. Effect of isothermal aging on the microstructural evolution in Ti-6Al-4V titanium alloy: experimental investigation and thermokinetic simulation

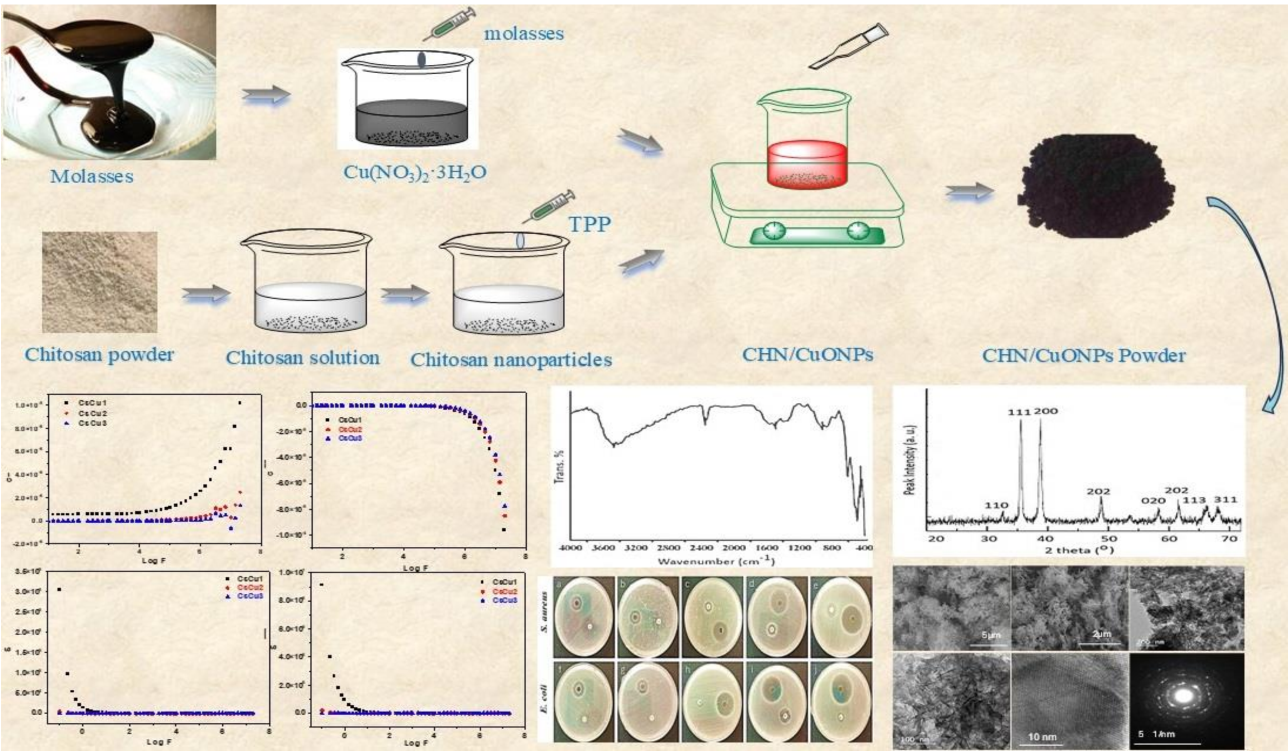
Nabil Kherrouba *, Walid Bedjaoui, Malek Hebib, Idir Hadji
Research Center in Industrial Technologies CRTI, P. O. BOX 64, Cheraga 16014, Algiers, Algeria

The precipitation mechanism and kinetics of the secondary α phase during short time duplex heat treatment and continuous cooling of the Ti-6Al-4V alloy were studied. The isothermal precipitation kinetics was determined using in-situ isothermal electrical resistivity tests in a Gleeble thermomechanical machine in the temperature range of 600-700°C. The results showed that the higher the aging temperature the faster the secondary α phase precipitation. The precipitation process was also investigated by simulation using the thermokinetic software MatCalc. Results of the simulation indicated that the secondary α phase nucleation ended at an earlier stage of the precipitation and that the latter is mainly controlled by the growth of secondary α phase precipitates. Evolution of the simulated elements contents showed that only the vanadium concentration in the β phase changed significantly during the isothermal aging. Thus, the growth of the secondary α phase is governed by the vanadium diffusion into the β phase. Besides, the transformation kinetics during cooling were investigated using the Differential Scanning Calorimetry. An approach based on the KJMA model has been developed and applied to determine the kinetics parameters. In both isothermal and non-isothermal conditions, a value of the Avrami index n=1 is obtained.

P12. Chitosan nanoparticles included different doses of copper oxide nanoparticles produced by molasses: Investigating electrical conductance and antibacterial attributes

Noof A. Alenazi *
Department of Chemistry, College of Science and Humanities in Al-Kharj, Prince Sattam bin Abdulaziz University, Al-kharj 11942, Saudi Arabia
* *+966594227188, na.alenazi@psau.edu.sa*

This research explores an environmentally friendly approach for synthesizing copper oxide nanoparticles (CuONPs) using molasses, which is rich in carbohydrates, polyphenols, and other beneficial compounds. This method eliminates the need for harsh processing conditions. The CuONPs were integrated into ionotropic chitosan nanoparticles (CsNPs) at varying concentrations, demonstrating effective production of small, stable CuONPs. The findings highlight the crucial role of CsNPs in maintaining CuONPs stability, preventing their aggregation into larger particles. An analysis revealed that both the dielectric constant and dielectric loss decreased with increased frequency, while a clear correlation was established between CuONPs and improved electrical conductivity. Additionally, the CsNPs-CuONPs nanocomposite exhibited antimicrobial properties against Escherichia coli (*E.coli*) and Staphylococcus aureus(*S. aureus*), showcasing its potential for biomedical applications. This technique provides a sustainable method for producing CuONPs-infused CsNPs without the use of organic solvents, costly raw materials, or complex machinery. Overall, this approach is notable for its effectiveness, simplicity, versatility, and cost-effectiveness, offering a safe and environmentally benign way to generate nanoparticles without contamination risks.



References

[1] G. Masoudi, M. Montazer, N. Ezazshahabi, A. Mianehro, M. Mahmoudirad, Biocompatible antibacterial denim fabric prepared via green synthesis of the copper oxide nanoparticles using raw sugar molasses, *Starch-Stärke* 74(9-10) (2022).

[2] 2. Nieto-Maldonado, S. Bustos-Guadarrama, H. Espinoza-Gomez, L.Z. Flores-López, K. Ramirez-Acosta, G. Alonso-Nuñez, R.D. Cadena-Nava, Green synthesis of copper nanoparticles using different plant extracts and their antibacterial activity, *Journal of Environmental Chemical Engineering* 10(2) (2022).

[3] S. Hemmati, S. Ahany Kamangar, A. Ahmeda, M.M. Zangeneh, A. Zangeneh, Application of copper nanoparticles containing natural compounds in the treatment of bacterial and fungal diseases, *Applied Organometallic Chemistry* 34(4) (2020).

[4] M.Z. Islam, Y. Fu, H. Deb, M.K. Hasan, Y. Dong, S. Shi, Polymer-based low dielectric constant and loss materials for high-speed communication network: Dielectric constants and challenges, *European Polymer Journal* 200 (2023).

[5] M. El-Morsy, N.S. Awwad, H.E. Ali, A. Menazea, Optical, thermal and dielectric properties of Copper Oxide (CuO)/chitosan (CS)/Polyethylene oxide (PEO) blends, *Journal of Polymer Research* 29(5) (2022).

P13. Investigation of local friction and surface potential properties of copper and mild steel under corrosion by atomic force microscopy

Igor Bdikin[1,2,*], Ricardo Beja[1,2], António Pereira[1,2]

[1] *TEMA: Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal*

[2] *LASI—Intelligent Systems Associate Laboratory, Guimarães, Portugal*

* bdikin@ua.pt

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

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

This work was developed in the scope of the Project “Agenda ILLIANCE” [C644919832-00000035 | Project no. 46], “AM2R – Agenda Mobilizadora para a inovação empresarial do setor das Duas Rodas” [C644866475-00000012 – project n. 15], and “ATE-Aliança para a Transição Energética” [C644914747-00000023| Project nº 56], financed by PRR – Recovery and Resilience Plan under the Next Generation EU from the European Union. This work also was supported: project UID 00481 Centre for Mechanical Technology and Automation (TEMA); and CENTRO-01-0145-FEDER-022083 - Centro Portugal Regional Operational Programme (Centro2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund.

P14. Antibacterial effect of ginger oil extract fixed in fluorohydroxyapatite

Maissa AGSOUS, Hafit KHIREDDINE, Sabeha YALA
Faculty of Technology, University of Bejaia, Targa Ouzemour, Algeria
* *213 674665089,* hafit.khireddine@univ-bejaia.dz

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

P15. Application of magnetic TiO2 /Carbon Quantum Dots composites for the photocatalytic removal of antibiotics from water

Valentina Silva[1, *], **Nuno J. O. Silva**[2], **Goreti Pereira**[1], **Marta Otero**[3], **Vânia Calisto**[1], **Diana L. D. Lima**[4]
[1] CESAM & Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal
[2] Department of Physics & CICECO, University of Aveiro, 3810-193 Aveiro, Portugal
[3] Departamento de Química y Física Aplicadas, Universidad de León, 24071 León, España
[4] H&TRC - Health & Technology Research Center, Coimbra Health School, Polytechnic University of Coimbra, 3046-854 Coimbra, Portugal
[*] Telephone: 234370360 and e-mail address: valentinagsilva@ua.pt

Antibiotics are essential in the global healthcare system. However, their presence in the aquatic environment, which is well documented, is harmful to ecosystems and promotes antimicrobial resistance. Such presence is largely related to wastewater treatment plants inefficiency for antibiotics removal. In the search for effective solutions, new treatments are being studied, including the application of solar-driven photocatalysis. This work aimed at optimizing the synthesis of a novel magnetic TiO_2/Carbon Quantum Dots (CQD) photocatalyst using a co-precipitation methodology. For this purpose, a Full Factorial Design (FFD) with 2 factors at 3 levels was used. The Fe:Ti and the CQD:TiO_2 *w/w* ratio were the studied factors and the photocatalytic removal (%) of the antibiotics (amoxicillin, sulfamethoxazole, and trimethoprim) under simulated solar radiation, together with results from vibrating sample magnetometry (VSM) and synthesis yield were the selected FFD responses. Considering these responses, and using Response Surface Methodology and Desirability function, it was found that the optimal combination of factors was 1.2:1 Fe:Ti and 4.0% CQD:TiO_2 *w/w* ratios. The so-synthesized nanocomposite was tested to compare the obtained with the predicted results for the FFD responses (photocatalytic removal of the target antibiotics, VSM and synthesis yield). Also, to assess its practical application, the effects of photocatalyst dosage (100 to 1000 mg L^{-1}) and pH (6 to 9) on the antibiotics' removal were tested. Results demonstrated that, the synthesized nanocomposite was as efficient as predicted for the removal of the three antibiotics. Furthermore, under the considered experimental conditions, its photocatalytic performance was maximum at a 500 mg L^{-1} dosage and satisfactory within the studied pH range. The obtained results are an excellent starting point for the development of a sustainable solution for the removal of antibiotics from water using magnetic TiO_2/CQD photocatalysts.

P16. Using $CuBiO_4/CuO$ Photocathodes to Avoid Hydrogen Evolution and Promote CO_2 Reduction in a Glycerol Microfluidic Fuel Cell

Maria-Victória S. Silva, [a] Silvio M. Mazarin,[a] Daniel F. Costa-Filho, [a] Adailton C. Nogueira, [a] Heberton Wender, [a] Cauê A. Martins [a]

[a] *Institute of Physics, Universidade Federal de Mato Grosso do Sul, CP 549, 79070-900, Campo Grande, MS, Brazil;*
+55 (067) 99207-0423, victoria.silva@ufms.br

Abstract

This study presents the development of a hybrid microfluidic fuel cell (μPFC) that converts glycerol and carbon dioxide (CO_2) into electrical energy. The central innovation lies in the integration of 3D-printed components with glass sealing, allowing precise control of reagent flow and the use of photosensitive catalysts. The anode uses Pt/C dispersed on carbon paper (CP) for the electrochemical oxidation of glycerol, while the photocathode consists of $CuBiO_4/CuO/CP$, facilitating CO_2 reduction under solar light exposure. The results demonstrate that the formation of the $CuBiO_4/CuO$ heterojunction effectively suppresses water splitting, preventing hydrogen bubble formation that could disturb laminar flow within the cell. The μPFC achieved a maximum power density of 0.9 mW cm^{-2}, indicating its potential as a sustainable solution for CO_2-to-energy conversion.

Introduction

The growing concern over CO_2 emissions has driven the search for efficient methods to capture and convert this gas into useful forms of energy [1]. Microfluidic fuel cells (μPFCs) have emerged as a promising approach, offering advantages such as enhanced mass transport efficiency and flexible design [2-3]. The integration of photosensitive catalysts in μPFCs allows for the utilization of solar light to drive electrochemical reactions, enhancing CO_2 conversion into electrical energy [4]. However, challenges such as concurrent water splitting and hydrogen bubble formation must be overcome to ensure the stability and efficiency of these systems.

Methodology

The μPFC developed in this study incorporates 3D-printed components with glass sealing, providing operational stability and enabling exposure of the photocatalytic components to light. The anode is composed of Pt/C dispersed on CP, responsible for glycerol oxidation in an alkaline medium. For the cathode, $CuBiO_4/CP$ and $CuBiO_4/CuO/CP$ electrodes were evaluated for CO_2 reduction at neutral pH under solar illumination. Electrochemical measurements, including cyclic voltammetry and polarization curves, were performed to assess the photoactivity of the electrodes and the cell's performance.

Figure 1

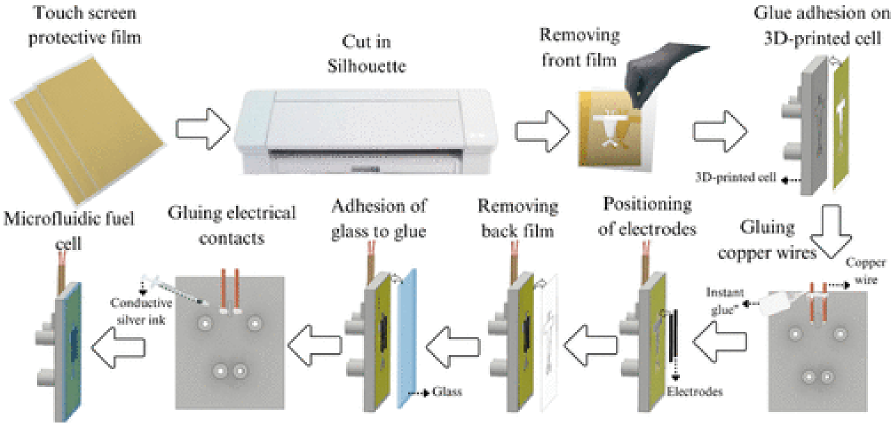


Figure 1. Details of the μPFC assembly, featuring all steps from cutting the touchscreen protective film to the placement of electrodes and sealing. Reprinted from [2].

Results

Half-cell measurements revealed that $CuBiO_4$/CP and $CuBiO_4$/CuO/CP electrodes exhibited significant photoactivity for CO_2 reduction under light exposure. The formation of the $CuBiO_4$/CuO heterojunction was effective in suppressing water splitting, minimizing hydrogen bubble generation and maintaining the integrity of laminar flow within the μPFC. The cell equipped with the $CuBiO_4$/CuO/CP photocathode achieved a maximum power density of 0.9 mW cm^{-2}, indicating efficient CO_2-to-energy conversion.

Figure 2

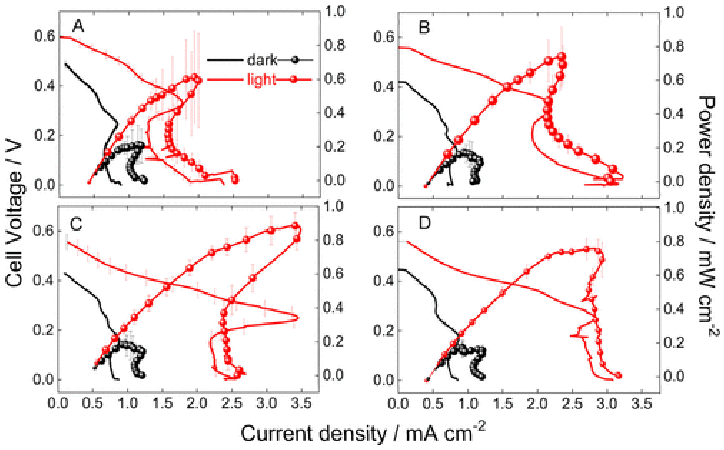


Figure 2. Polarization and power density curves of a μPFC equipped with a CBO/CuO/CP photocathode and Pt/C/CP dark anode fed by 1 mol L^{-1} glycerol + 1 mol L^{-1} KOH anolyte and CO_2-saturated PBS catholyte at (a) 30, (b) 50, (c) 75, and (d) 100 μL min^{-1}. Measurements were collected from the OCV to 0.01 at 0.01 mV s^{-1} under light induced by a solar simulator at 200 mW cm^{-2}. Reprinted from [2].

Discussion

The suppression of water splitting by the $CuBiO_4$/CuO heterojunction is a significant advancement, as hydrogen bubble formation can compromise the operational stability of μPFCs. The integration of 3D-printed components with glass sealing not only ensures the mechanical stability of the cell but also facilitates the exposure of photocatalysts to light, maximizing the efficiency of photoelectrochemical reactions. Furthermore, using glycerol as fuel at the anode represents a sustainable approach, utilizing a byproduct of the biodiesel industry for clean energy generation.

This study demonstrates the potential of μPFCs equipped with $CuBiO_4$/CuO photocathodes for efficient CO_2-to-energy conversion, offering a promising solution for mitigating greenhouse gas emissions and promoting sustainable energy technologies.

Conclusions

This μPFC efficiently converts CO_2 and glycerol into energy, achieving 0.9 mW cm^{-2} power output. It demonstrates a significant step toward sustainable energy solutions with further research potential.

References

[1] N. Khan, F. Stelo, G. H. C. Santos, L. M. Rossi, R. V. Gonçalves, and H. Wender, Applied Surface Science Advances, **11**, 100289 (2022).
[2] S. M. Mazarin, D. F. Costa-Filho, C. R. Zanata, A. C. Nogueira, M. V. S. Silva, H. Wender, and C. A. Martins, *ACS Omega*, **9**, 43658-43667 (2025).
[3] C. R. Zanata, M. J. M. Zapata, H. Wender, and C. A. Martins, *Electroanalysis*, **36**, 202400214 (2025).
[4] B. D. Queiroz, J. A. Fernandes, C. A. Martins, and H. Wender, Journal of Environmental Chemical Engineering, **10**, 107611 (2022).

P17. Eco-Friendly Synthesis of Iron Oxide Nanoparticles and Their Application to the Removal of Arsenic and Lead from Mining-Contaminated Soils

Erico Carmona[1,*], Aliro Villacorta[1], Felipe Carevic[1], Lucas Hernández[1], Cynthia Rojo[1], Ricard Marcos[2]

[1]*Arturo Prat University, Renewable Natural Resources Faculty, Huayquique Campus, 1100000, Iquique, Chile*

[2]*Universitat Autònoma de Barcelona, Departamento de Genetica i de Microbiología, 08193 Bellaterra (Cerdanyola del Valles), Spain*

[*] *+56 973894115, ecarmona@unap.cl*

There are different synthesis methods of metal oxide nanoparticles (NPs); however, green synthesis can be considered one of the most promising methodologies since it is simple, low-cost, ecological, non-toxic, and generates stable NPs, which makes it a promising methodology for scaling up [1,2]. Green synthesis involves NPs from mixing metal salts and natural agents such as vitamins, sugars, plant extracts, biodegradable polymers, and microorganisms. When plant extracts are used, they can act as a reducing agent and stabilizing component for the system [3]. Iron NPs synthesized by the green route have excellent properties for removing heavy metals from soil and water [4]. Thus, this nanomaterial can be considered a good candidate for fabricating advanced materials to clean polluted environments of heavy metals.

This paper reports on developing an eco-friendly method for synthesizing magnetite and Fe oxide NPs. The use of Fe recovered from tailing ores was studied, as well as the use of iron commercial salts ($FeCl_3$ and $FeSO_4$) as raw materials. Likewise, fruit peel waste and plant extracts were used as bio-reducing and stabilizing agents for the green process. Fe NPs were physically characterized using UV-Vis, FTIR, XDR, SEM, TEM, AFM, DLS, and LDV techniques. In addition, Fe NPs were investigated for immobilizing hazardous metals from soil samples polluted by heavy metals. The results indicated the formation of Fe oxide and Magnetite NPs with sizes ranging from 4 to 30 nm, rod-like shape, crystallinity, and stable hydrodynamic behavior. Based on FTIR analysis, the mechanism synthesis suggested could be related to the presence of polyphenols of vegetal extracts that can reduce the metal ions to form nucleation and stable nanoparticles in the process. Batch experiments incubating soils with 5% and 10% p/p of magnetite NPs obtained by green synthesis showed significant simultaneous immobilization of lead and arsenic metals from polluted soil samples. Lead was immobilized at around 60%, while Arsenic was almost 100% removed from soil samples. Also, a neutralizing effect of the pH of soils treated with magnetite nanoparticles was observed in the experiments.

References

[1] Soltys, L., Olkhovyy, O., Tatarchuk, T., & Naushad, M. (2021). Green synthesis of metal and metal oxide nanoparticles: Principles of green chemistry and raw materials. Magnetochemistry, 7(11), 145.

[2] Sahoo, K., & Kumar, S. (2021). Green synthesis of sub 10 nm silver nanoparticles in gram scale using free impinging jet reactor. Chemical Engineering and Processing-Process Intensification, 165, 108439.

[3] Carmona, E. R., Benito, N., Plaza, T., & Recio-Sánchez, G. (2017). Green synthesis of silver nanoparticles by using leaf extracts from the endemic Buddleja globosa hope. Green Chemistry Letters and Reviews, 10(4), 250-256.

[4] Bolade, O. P., Williams, A. B., & Benson, N. U. (2020). Green synthesis of iron-based nanomaterials for environmental remediation: A review. Environmental Nanotechnology, Monitoring & Management, 13, 100279.

P18. Thermal Analysis of TIG Welding: Experimental Study and Comparison with FE and FD Numerical Methods

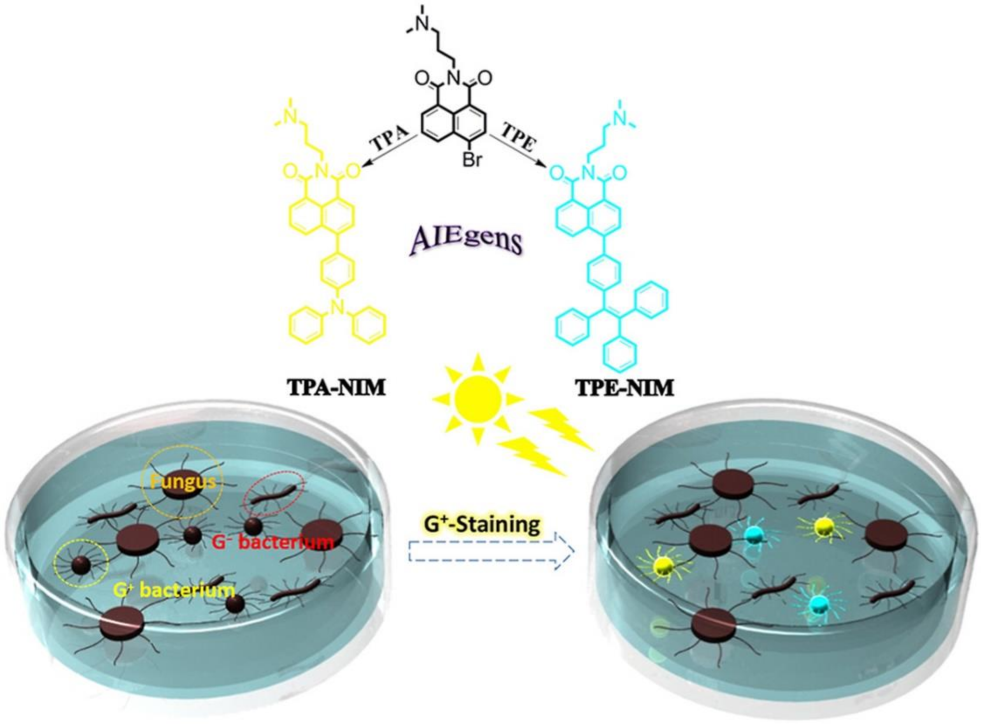
Abdel Halim Zitouni [1, *], Mouloud Aissani [1], Pierre SPITERI [2], Younes Benkheda[3]
[1]Research Center in Industrial Technologies CRTI P.O.BOX 64, Cheraga 16014 Algiers, Algeria
[2]IRIT, INP-ENSEEIHT, 2 Rue Charles Camichel 31000, Toulouse, France
[3]Département de Génie Mécanique, Université de Blida1, BP 270, Route de Soumaa, Blida, Algérie
**a.zitouni@crti.dz*

This work presents a thermal analysis of the TIG (Tungsten Inert Gas) welding process. In the experimental phase, 304L stainless steel sheets were welded and thermal cycles at various locations were recorded using thermocouples. The second phase involved developing a mathematical model to describe the heat flux generated by the TIG arc welding process without filler metal. Two numerical methods were used to implement this model: the first employed a Finite Difference (FD) approach using a custom FORTRAN program, while the second utilized the Finite Element (FE) method via COMSOL Multiphysics. The main objective was to compare the experimental data with the results from both numerical approaches to evaluate the accuracy, strengths, and limitations of each. The resulting heat distribution calculations enabled the identification of critical regions affected by the welding process, including the Heat-Affected Zone (HAZ) and the Melted Zone (MZ).

P19. AIE-Active Nanoprobes for Rapid and Selective Fluorescence Identification of Gram-Positive Bacteria

Arshad Khan*, Ibraheem Bushnak, Rizwan Ali
Nanomedicine Department & core facility, King Abdullah International Medical Research Center (KAIMRC) King Saud Bin Abdulaziz University for Health Sciences, Riyadh 11426, Kingdom of Saudi Arabia
* *Phone: 00966505722694, Email: khanar@kaimrc.edu.sa*

Rapid and accurate differentiation between Gram-positive (G^+) and Gram-negative (G^-) bacteria is critical for effective clinical diagnosis and antimicrobial therapy. In this work, we present two naphthalimide-based luminogens—tetraphenylethylene-naphthalimide (TPE-NIM) and triphenylamine-naphthalimide (TPA-NIM)—which exhibit strong aggregation-induced emission (AIE) properties and exceptional selectivity toward G^+ bacteria. These AIE-active bioprobes enable wash-free, fluorescence-based tracking of six bacterial species and two fungal strains, displaying a clear preference for G^+ bacteria over G^- and fungal cells. Beyond planktonic cells, both probes effectively visualize G^+ bacterial biofilms and successfully track Staphylococcus aureus in red blood cell suspensions, demonstrating practical utility in complex biological environments. Mechanistic investigations suggest that electrostatic and hydrophobic interactions synergistically drive the selective binding. With their low toxicity, robust photostability, and high imaging specificity, TPE-NIM and TPA-NIM represent promising tools for pathogen detection and pave the way for new theranostic applications of AIE-based materials in infectious disease management.These results highlight their value as versatile nanodiagnostic tools for infectious disease monitoring.



P20. A comparison of HPPC and PEIS test methodology for determination of LFP cells performance

Marko Viskić[1, *], Željko Ban[2], Zoran Mandić[1]

[1]*Department of Electrochemistry, Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10000 Zagreb, Croatia*

[2]*Department of Control and Computer Engineering, Faculty of Electrical Engineering and Computing, University of Zagreb, Unska 3, 10000 Zagreb, Croatia*

* +385 1 4597 117, mviskic@fkit.ht

Nowadays, LFP (lithium ferro-phosphate) Li-ion batteries are widely targeted for use in grid-scale energy storage, electric vehicles, and solar energy installations, owing to the exceptionally long cycle life and improved safety when compared to other Li-ion chemistries.[1] As SoC and SoH values are crucial for estimating battery performance, the methods used for their determination based on real physical models are being developed. Hereby, EIS (Electrochemical Impedance Spectroscopy) and HPPC (hybrid pulse power characterization) were applied to determine the parameters of commercial IFR 18500 batteries. HPPC tests were carried out by charging the batteries and applying discharge-charge pulses of constant duration with three different current values at battery SoC ranging between 90% and 10%. Rest periods were applied after 10% discharge periods as well as between the individual pulses. The EIS measurement was done concurrently, during the HPPC rest phase. Based on a Thevenin model, a cell equivalent circuit was designed. Identification of the circuit parameters was done in EC-Lab software for the EIS measurements, while for the HPPC, a custom application was written in the MATLAB/Simulink environment. The results have shown a good correlation between techniques for the determination of some parameters, as well as a stable trend between the circuit resistances and SoC of the battery based on the duration and power of the pulse. Improvement of the equivalent circuit has to be done due to the influence of diffusion taking place for current pulses of longer duration.

This work was financially supported by the project “Advanced innovative materials and technologies for lithium-ion batteries production.”, NPOO.C3.2.R3-I1.04.0187

References

[1] H.C. Chung, T.D.H. Nguyen, S.Y. Lin, W.B. Li, N.T.T. Tran, N. Thi Han, H.Y. Liu, H.D. Pham, L. Hai Duong; M.F. Lin, *Engineering integrations, potential applications, and outlooks of Li-ion battery industry,* in: *First-Principles Calculations for Cathode, Electrolyte and Anode Battery Materials*, IOP Publishing, Bristol, UK, (2021).

P21.Self-trapped Polaron Signatures In Ligand-assisted Lead Halide Perovskite Nanocrystals

S. K. Jakka[1]*, **T. Udaybaskarrao**[2], **R. Vidyasagar**[3]*

[1] I3N & Department of Physics, University of Aveiro, Aveiro 3810-193, Portugal
[2] Institute of Fundamental and Frontier Sciences, UESTC, Chengdu 610054, China
[3] CICECO & Physics Department, University of Aveiro, Aveiro 3810-193, Portugal
* *E-mail: suresh@ua.pt; dr.vidyasagar79@gmail.com*

We report the spectroscopic observation of self-trapped polaron exciton signatures in ligand-assisted CsPbBr3-Cs4PbBr6 nanocrystals prepared by colloidal synthesis. The temperature dependence of photoluminescence spectrum measured with photo-excitation spectroscopy show broad shoulder emissions below the exciton signatures in visible wavelength region, which are attributed to the formation of self-trapped polaron exciton corresponding to the relaxation of electrons and holes sits on Pb23+, and Pb3+ sites, respectively. While self-trapped polaron exciton emission peaks shifted to lower energies side, its intensity substantially enhanced with decreasing temperature from T=180-14 K. The polaron excitons band shifting is attributed to the change of self-trapped electronic levels by the large exchange field of Pb-6p orbitals during relaxation process and vibrational lattice environment and; those self-trapped carriers act like non-radiative centers for deteriorating exciton intensity. The presentation will include a general introduction to glasses and their properties, an overview of PL through various dopants, and a discussion on different PL mechanisms. It will also cover the fabrication of glasses and fibers, especially chalcogenide glasses, and detail the mechanisms of gas detection using these advanced materials.

Acknowledgements: This work is financed by national funds through FCT - Fundação para a Ciência e a Tecnologia, I.P. and the Ministry of Science, Technology and Higher Education under project LA/P/0037/2020, UIDB/50025/2020, UIDP/50025/2020. S. K. Jakka acknowledges the funding by national funds through FCT – Portugal, I.P., in the scope of the framework contract foreseen in the numbers 4, 5 & 6 of article 23, of the Decree-Law 57/2016, of August 29, changed by Law 57/2017, of July 19. This work was partially supported by the project i3N, UIDB/50025/2020 & UIDP/50025/2020, financed by national funds through the FCT/MEC. Udayabhaskar Thumu acknowledges financial support provided by the NSFC Grant No. 22050410280 and UESTC grants. R. Vidyasagar thanks Fundação para a Ciência e Tecnologia, Portugal (FCT-Portugal) for the Grant SFRH/BPD/104887/2014.

2nd Workshop on High Valued Developments in Photocatalysis

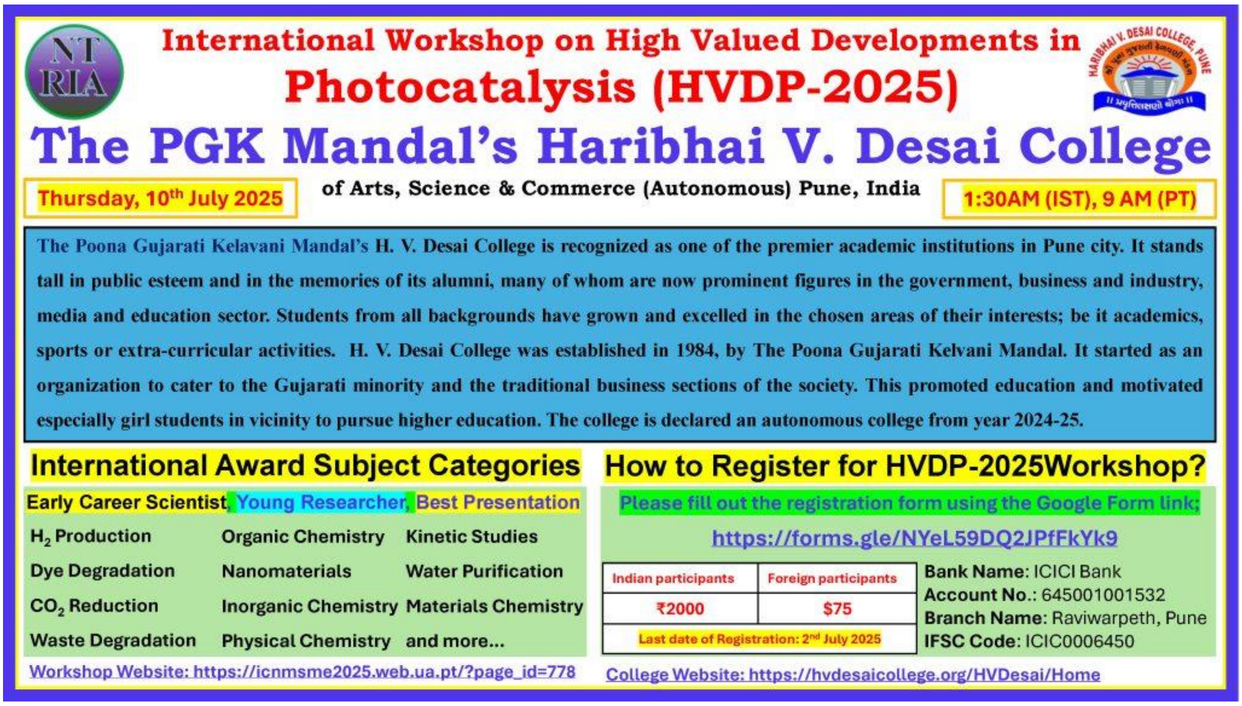
International Workshop on

High Valued Developments in Photocatalysis [HVDP-2025]

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

Thursday, 10th July, 2025

Time: 1:30 pm



International Workshop on High Valued Developments in Photocatalysis (HVDP-2025)

The PGK Mandal's Haribhai V. Desai College

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

Thursday, 10th July 2025

1:30AM (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.

International Award Subject Categories

Early Career Scientist, Young Researcher, Best Presentation

H_2 Production
Dye Degradation
CO_2 Reduction
Waste Degradation
Organic Chemistry
Nanomaterials
Inorganic Chemistry
Physical Chemistry
Kinetic Studies
Water Purification
Materials Chemistry
and more...

How to Register for HVDP-2025Workshop?

Please fill out the registration form using the Google Form link;

https://forms.gle/NYeL59DQ2JPfFkYk9

Indian participants	Foreign participants
₹2000	$75
Last date of Registration: 2nd July 2025	

Bank Name: ICICI Bank
Account No.: 645001001532
Branch Name: Raviwarpeth, Pune
IFSC Code: ICIC0006450

Workshop Website: https://icnmsme2025.web.ua.pt/?page_id=778

College Website: https://hvdesaicollege.org/HVDesai/Home

WHVDP-2025 focuses on Great achievements in Photocatalysis field to generate Hydrogen Gas and to clean the organic toxic wastes. Semiconductor Nanostructured materials are well known in the field of Photocatalysis.

Topics:

Photocatalytic Hydrogen Production
Photocatalytic Water Splitting
Photocatalytic Dye Degradation
Photocatalytic Waste Degradation
Photocatalytic Toxic Compounds Degradation
High Valued Developments in Photocatalysis
Photocatalytic Applications

Our Strength

Shri. Rajeshbhai Shah
Chairman
The PGK Mandal Pune

Shri. Hemantbhai Maniar
Secretary
The PGK Mandal Pune

Shri. Dilipbhai Jagad
Joint Secretary
The PGK Mandal Pune

Conveners of WHVDP-2025:

Dr. Vikram U. Pandit
Assistant Professor
(Haribhai V. Desai College, Pune, India)

Dr. Rajendra G. Gurao
Principal
(Haribhai V. Desai College, Pune, India)

The Poona Gujarati Kelwani Mandal, Pune

Shri. Rajesh Shah, Chairman
Shri Janak Shah, Vice-Chairman
Shri. Hemant Maniar, Secretary

Shri. Vinod Dedhia, Joint Secretary
Shri. Mahesh Dharod, Treasurer
Shri. Kantilal Patel, Joint Treasurer
Shri. Dilip Jagad, Joint Secretary
Shri. Pramod Shah, Joint Secretary
Shri. Sandeep Shah, Joint Secretary

Scientific committee:
Dr. Prakash Wadgaonkar (Pune, India)
Dr. Sudhir Arbuj (Pune, India)
Dr. Dattatreya Late Pune, India
Dr. Gusavo Colpani (Chapeco, Brazil)
Dr. Dalila Hammiche (Bejaia, Algeria)
Dr. Shivaji Pandit (Ahmednagar, India)
Dr. Pramod Kamble (Rjasthan, India)
Dr. Alaa Ghidan (Jordan)
Dr. Satish Meshram (Amravati, India)
Dr. Swapnil Sonawane (New Delhi, India)
Dr. Pratik Nagawade (Ahmednagar, India)
Dr. Yashwant Pandit (Israel)
Dr. Alaa Alasadi (Karbala, Iraq)
Dr. Vivek Jawale (Pune, India)
Dr. Yashpal Rathod (Bhandara, India)
Dr. Pradip Kate (Solapur, India)
Dr. Aeed Fahdawi (Iraq)
Dr. Ramdas Huse (Buldana, India)
Dr. Asaad Abd Al-Hussien (Iraq)

Organizing committee:

Dr. Rajendra Gurao (Pune, India)
Dr. Vikram Pandit (Pune, India)
Prof. Omkar Malusare (Pune, India)
Prof. Ganesh Jadhav (Pune, India)

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

Workshop Contact: vikramupandit@gmail.com, vikram.pandit@hvdesaicollege.co.in

Workshop Website: https://icnmsme2025.web.ua.pt/
https://icnmsme2025.web.ua.pt/?page_id=778

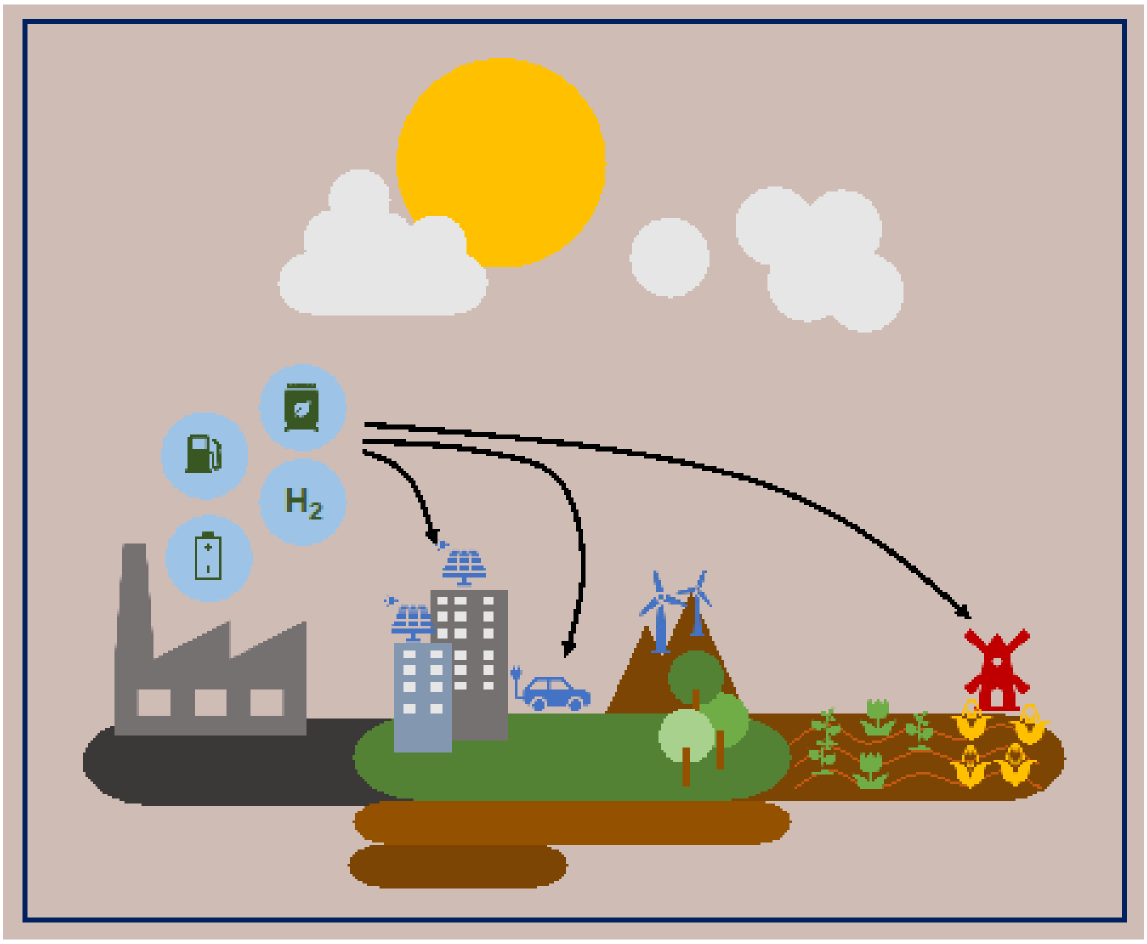
HVDP 2025

Time	**Name of Speaker**	**Topic**
9:00: 9:05	**Dr. Vikram Pandit-** Introduction to Workshop	
9:05: 9:10	**Dr. Igor Bdikin** Welcome on behalf of Conference	
9:10: 9:15	**Dr. Rajendra Gurao,** Principal, Welcome of all participants	
9:15: 9:40	**Dr. Vivekanand Jawale** Keynote Speaker Topic: Dual-Functional Zinc Oxide Nanostructures: Harnessing Environmental Remediation and Antioxidant Potential through Ag-Embedded Composites	
Oral Presentations		
9:40-9:50	Dawange Ganesh Punjaba	Green synthesis of copper oxide nanocatalyst using plant extract and its antibacterial and photocatalytic applications
9:50-10:00	Beg Waseem Ahamad	"A Colorimetric Detection Probe for Al(III) by phenolphthalein hydrazone Schiff Base"
10:00-10:10	Tushar Mahadev Patil	Graphitic Carbon Nitride: Effect of various precursors on dye degradation and drug degradation
10:10-10:20	Ms.Rohini Baban Thakare	Recent Advances in the Synthesis and Characterization of Schiff Base Ligands and Their Metal Complexes: A Pathway to Functional Materials"
10:20-10:30	Thombare Sakshi Shamrao	6,13-Pentacenequinone and 5, 7, 12, 14-Pentacenetetrone for Photocatalytic Applications
10:30-10:40	Purnima Mallikarjun Patil	Enhanced Photocatalytic Degradation of Methylene blue using SnO 2- PQ nanocomposite
10:40-10:50	Bhagwan Daphal	Polyaniline: Robust Green Light-Driven Photocatalyst for Multi-Textile Dye Degradation
10:50-11:00	Mithari Jatin Abhay	Pentacenequinone/BiOI (BiOX, X = I) Photocatalyst for Dye Degradation.
11:10-11:20	Ganesh Jadhav	Synthesis, Characterization of Pr(OH)3 Nanowires for Enhanced Photocatalytic Activities
11:20-11:30	Kavita Mahaveer Durgade	Synthesis and Characterization of nitrogen containing heterocyclic Quinazoline Derivatives.
11:30-11:40	Bhalerao Priyanka Ganesh	Synthesis and characterisation of transition metal sulphide nanoparticles as an efficient photo & electrocatalyst for efficient Hydrogen evolution

4th International Workshop on "Modern Trends in Energy Research"

WMTER-2025

July 10, 2025, Aveiro, Portugal



Topics:

Green Hydrogen: Production, Storage & Transport

Fuel Cells/Electrolysers

Electrochemical Synthesis of Green Fuels and Chemicals

Batteries & Supercapacitors

Nanocatalysis & Electrocatalysts

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

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

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

Local Organizing committee:

Dr. D. Pukazhselvan (UA, Portugal)
Dr. 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 2025

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

Length of each lectures:
15 minutes + additional 5 minutes for Q&A.

4th International Workshop on Modern Trends in Energy Research

(In association with 7th International Conference on Nanomaterials Science and Mechanical Engineering: ICNMSME-2025)

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

10th July 2024, 14 h to 16h h

Session:1

Chair: Francisco Loureiro (Co-convener, WMTER 2025)

14.00 – 14.05	**Workshop introduction and welcome Address** **D. Pukazhselvan (Convener WMTER 2025)**
14.05 – 14.40	**Plenary Lecture** **Fausthon Fred da Silva** Department of Chemistry, Federal University of Paraíba, Brazil ***Title: "Phyto-mediated green synthesis of NiO nanoparticles for OER electrocatalysis"***
14.40 – 15.00	**Keynote Address** **Ihsan Çaha** International Iberian Nanotechnology Laboratory, Braga, Portugal ***Title: "Ultrafast Transmission Electron Microscopy: A New Frontier for Dynamic Imaging at the Nanoscale"***

Session:2

Chair: Vanessa Graca

15.00 – 15.20	**Invited Talk-1** **Allan J. M. Araújo** TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal ***Title: "Layered Ruddlesden–Popper lanthanum nickelates for SOC oxygen electrodes: Effect of PrOx impregnation"***
15.20 – 15.40	**Invited Talk-2** **Paula Rosendo Santos** Facultad de Farmacia, Departamento de Química y Bioquímica, Urbanización Monteprincipe, Universidad San Pablo-CEU, CEU Universities, E-28668 Madrid, Spain ***Title: "Unveiling the Mechanism of Exsolution of Silver Nanoparticles for Decorating Lanthanum Strontium Ferrite and assessment of its electrochemical behavior"***

15.40 – 16.00	**Invited Talk-3** **Jayakrishnan K. Ravindran** TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal ***Title: "Environmental Assessment of MSW-to-FT Fuel Pathways: Impact of Gasification and Tail Gas Utilization Strategies"***
16.00 – 16.20	**Invited Talk-4** **Carlos O Amorim** Department of Physics and i3N, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal **Title: "Low-Temperature, Rapid Synthesis of Cu3BiS3 Thin Films for Sustainable Photovoltaics"**
16.20 – 16.30	**Session break**

Session:2

Chair: Laura Holz

16.40 – 17.00	**Invited Talk-5** **Jaykumar Lachure** Department of Computer Engineering & Information Technology, VJTI Mumbai, India **Title: "Quantum-Informed Generative Optimization (QIGO) for Catalyst-Free Hydrogen Evolution Using Hybrid Quantum-AI"**
17.00-17.20	**Invited Talk-6** **Morena B. Farias** Department of Materials Science and Engineering Postgraduate Program, Federal University of Rio Grande do Norte, Brazil ***Title: "Improvement of cobalt-free perovskite electrodes for application in solid oxide fuel cells"***
17.20 – 17.40	**Invited Talk-7** **Raquel Dantas** Department of Chemistry, CICECO-Aveiro Institute of Materials, University of Aveiro, Portugal ***Title: "From Design to Performance: Redox-active COFs as advanced organic electrode materials"***
17.40-17.55	**Invited Talk-8** **D. Pukazhselvan** TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Portugal ***Title: "Reactive Hydride Composites: A Promising Pathway for High-Capacity Hydrogen Storage"***
17.55-18.00	**Vote of Thanks/Concluding remarks**

Plenary Lecture

Phyto-mediated green synthesis of NiO nanoparticles for OER electrocatalysis

Giovani Luiz da Silva[1], Adiel Soares Ferreira[2], Johnnys da Silva Hortêncio[1] João Pedro Gonçalves de Souza Soares[3], Annaíres de Almeida Lourenço[1], Nykon Craveiro[4], Rafael A. Raimundo[5], Rubens Teixeira De Queiroz[6], José Souto Rosa Filho[4], Daniel Araújo Macedo[5], Fausthon Fred da Silva[2*]

[1] Departamento de Química, Universidade Federal da Paraíba (UFPB), 58.051-900, João Pessoa, PB, Brazil
[2] Programa de Pós-Graduação em Química, Universidade Federal Rural de Pernambuco (UFRPE), 52171-900, Recife, PE, Brazil.
[3] Programa de Pós-Graduação em Engenharia Química, Universidade Federal do Rio Grande do Norte (UFRN), 59078-970 Natal, RN, Brazil
[4] Laboratório de Bentos (LaBen), Departamento de Oceanografia, Universidade Federal de Pernambuco,50670-901 Recife-PE, Brazil.
[5] Programa de Pós-Graduação Em Ciência e Engenharia de Materiais - PPCEM, Universidade Federal da Paraíba (UFPB), 58.051-900, João Pessoa, PB, Brazil
[6] Departamento de Sistemática e Ecologia, Universidade Federal da Paraíba (UFPB), 58.051-900, João Pessoa, PB, Brazil
[*] fausthon@quimica.ufpb.br

Abstract: Global ecological imperatives underscore the need for clean, renewable energy sources such as hydrogen (H_2), a promising energy carrier primarily generated via water electrolysis.[1] Although this process is environmentally benign, its high energy demand necessitates the use of electrocatalysts to render it viable. Accordingly, significant research has focused on developing high-performance electrocatalysts based on earth-abundant transition metals. Greener synthesis pathways—particularly those employing plant extracts to stabilize nanoparticles—are also gaining traction because they help reduce environmental impact. Nanostructured transition-metal oxides, notably nickel oxide (NiO), display wide applicability, especially as electrocatalysts in energy-conversion devices.[2] Yet sustainable development demands environmentally compatible synthesis technologies for these oxides, especially for large-scale production. In this context, our group has used ethanolic extracts of plants (*Ipomoea asarifolia*) and algae (Sargassum spp.) as stabilizing agents to produce NiO nanoparticles at different calcination temperatures. The phytochemical composition of the plant extract was analyzed by HPLC, and the resulting materials were characterized XRD, FTIR, Raman, , solid-state UV–Vis spectroscopy, SEM-EDS and TEM. Electrocatalytic performance toward the oxygen evolution reaction (OER) in alkaline medium ($1.0\,\mathrm{mol\,L^{-1}}$ KOH) was assessed, yielding overpotentials of 307–405 mV at a current density of $10\,\mathrm{mA\,cm^{-2}}$; the samples synthesized with plant extracts showed the most favorable results. Moreover, the synthesis protocol proved highly reproducible and delivered electrocatalytic performance comparable to or better than analogous materials reported in the literature.

Acknowledgment: *Prof. Dr. Fausthon F. da Silva thanks the National Institute of Science and Technology on Molecular Sciences (INCTCiMol) and CNPq (406804/2022-2, 303521/2022-8).*

References

[1] *N. Armaroli e V. Balzani, ChemSusChem, 4 (2011), 21–36*
[2] *M. Plevová, J. Hnát, e K. Bouzek, J Power Sources, 507 (2021), 230072.*

Keynote Address

Ultrafast Transmission Electron Microscopy: A New Frontier for Dynamic Imaging at the Nanoscale

Ihsan Çaha

International Iberian Nanotechnology Laboratory (INL), Avenida Mestre Jose Veiga, Braga, Portugal
Ihsan.caha@inl.int

Capturing how materials evolve in both time and space is essential for unlocking the next generation of functional nanotechnologies. Traditional electron microscopy excels in spatial resolution but lacks the temporal resolution needed to observe fast, transient processes such as magnetization switching, charge redistribution, or lattice vibrations.[1] Ultrafast pulsed transmission electron microscopy (UFP-TEM) overcomes this barrier by combining nanometer-scale imaging with sub-nanosecond time resolution.[2]

In this talk, I will introduce recent advancements in UFP-TEM instrumentation and methodology, including RF-compatible MEMS platforms, stroboscopic imaging modes, and cryo-compatible sample environments. I will highlight how this emerging technique enables real-time observation of nanoscale dynamics across a wide range of systems, from low-dimensional magnets and ferroelectrics to energy conversion materials.

Examples will include imaging GHz-frequency spin textures, probing charge and strain dynamics in quantum-confined structures, and investigating curvature-driven phenomena in encapsulated materials. These studies demonstrate how ultrafast TEM provides new insight into structure–function relationships that were previously inaccessible.

This talk aims to provide a broad perspective on how temporal resolution is transforming transmission electron microscopy and why this shift matters for researchers working across condensed matter physics, nanomaterials, and device engineering.

Acknowledgment: *This work was supported by the Innovation Pact "NGS - New Generation Storage" (C644936001-00000045), by "NGS" Consortium, co-financed by NextGeneration EU, through the Incentive System "Agendas para a Inovação Empresarial" ("Agendas for Business Innovation"), within the Recovery and Resilience Plan (PRR).*

References

[1] Alcorn, F. M., Jain, P. K. & van der Veen, R. M. Time-resolved transmission electron microscopy for nanoscale chemical dynamics. *Nat. Rev. Chem.* **7**, 256–272 (2023).
[2] Liu, C. *et al.* Correlated spin-wave generation and domain-wall oscillation in a topologically textured magnetic film. *Nat. Mater.* **24**, (2025).

Invited Talk-1

W2-I1. Layered *Ruddlesden–Popper* lanthanum nickelates for SOC oxygen electrodes: Effect of PrO_x impregnation

Allan J. M. Araújo[1,2,*], **Morena B. Farias[3]**, **Carlos A. Paskocimas[3]**,
Duncan P. Fagg[1,2], **Francisco J. A. Loureiro[1,2]**

[1] *TEMA – Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal*
[2] *LASI – Intelligent Systems Associate Laboratory, 4800-058 Guimarães, Portugal*
[3] *Materials Science and Engineering Postgraduate Program – PPGCEM, Federal University of Rio Grande do Norte – UFRN, 59078-970 Natal, Brazil*
[*] *allan@ua.pt and allanjmaraujo@gmail.com*

Abstract: There are growing concerns about the environmental impact, health risks and long-term instability of cobalt- and strontium-based materials, which are commonly employed in oxygen electrodes for solid oxide cells (SOCs). These concerns are particularly related to the environmental and health issues associated with cobalt extraction, as well as the tendency of strontium to segregate and react with CO_2. In this context, cobalt- and strontium-free *Ruddlesden–Popper* (RP) phases, $La_2NiO_{4+\delta}$ (L2N1) and $La_4Ni_3O_{10-\delta}$ (L4N3), have emerged as promising alternatives. However, these materials still face challenges due to limited oxygen transport, as the diffusion process occurs predominantly *via* surface pathways during the oxygen reduction reaction (ORR) [1]. To address this, the effect of praseodymium oxide (PrO_x) nanoparticle impregnation on polarisation processes was evaluated. Of the two compositions, L2N1 exhibited superior performance due to greater ambipolar conductivity [2,3]. Following PrO_x infiltration, the polarisation resistance at 700 °C decreased significantly to ~0.6 Ω cm^2 for L2N1 and ~0.8 Ω cm^2 for L4N3, representing reductions by factors of ~7 and ~17, respectively. These improvements are attributed to enhanced surface kinetics and charge transfer processes catalysed by PrO_x. The results demonstrate that PrO_x-impregnated RP materials are a promising, stable and efficient alternative to SOC oxygen electrodes.

Acknowledgment: *The authors acknowledge the following grants/projects: 2020.02797.CEECIND/CP1589/CT0030 (https://doi.org/10.54499/2020.02797.CEECIND/CP1589/CT0030), PTDC/CTM-CTM/2156/2020 (https://doi.org/10.54499/PTDC/CTM-CTM/2156/2020), 2022.02498.PTDC (https://doi.org/10.54499/2022.02498.PTDC), COMPETE2030-FEDER-00770000, 2022.09319.PTDC (https://doi.org/10.54499/2022.09319.PTDC), UIDB/00481/2020 (https://doi.org/10.54499/UIDB/00481/2020) and UIDP/00481/2020 (https://doi.org/10.54499/UIDP/00481/2020) 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). This study was also financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – Brazil (CAPES) – Finance Code 001. Carlos A. Paskocimas acknowledges the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq/Brazil, 302887/2022-9).*

References

[1] N. Hildenbrand, P. Nammensma, D. H. A. Blank, H. J. M. Bouwmeester and B. A. Boukamp, J Power Sources, 2013, 238, 442–453.
[2] J. Song, D. Ning, B. Boukamp, J. M. Bassat and H. J. M. Bouwmeester, J Mater Chem A Mater, 2020, 8, 22206–22221.
[3] M. B. Farias, A. J. M. Araújo, C. A. Paskocimas, D. P. Fagg and F. J. A. Loureiro, Dalton Trans., 2024, 53, 16610–16620.

Invited Talk-2

W2-I2. Unveiling the Mechanism of Exsolution of Silver Nanoparticles for Decorating Lanthanum Strontium Ferrite and assessment of its electrochemical behavior

M. Teresa Azcondo[a]; Gloria Anemone[b]; Alvaro Muñóz-Noval[c]; Khalid Boulahya[d] ; Juan Rubio-Zuazo[e]; Paula Rosendo[a*]; Ulises Amador[a].

[a] Facultad de Farmacia, Departamento de Química y Bioquímica, Urbanización Montepríncipe, Universidad San Pablo-CEU, CEU Universities, E-28668 Madrid, Spain
[b] Departamento de Métodos Cuantitativos, CUNEF Universidad, Madrid 28040, Spain
[c] Departamento de Física de Materiales, Facultad de Físicas, Universidad Complutense, E-28040 Madrid, Spain; IMDEA Nanociencia, 28049 Madrid, Spain
[d] Departamento de Química Inorgánica I, Facultad de Ciencias Químicas, Universidad Complutense, 28040 Madrid, Spain
[e] SpLine Spanish CRG Beamline, ESRF, Grenoble, Isere/Rhone-Alpes 38042, France; Instituto de Ciencia de Materiales de Madrid-ICMM/CSIC, Madrid 28049, Spain
[*] paula.rosendosantos@ceu.es

Abstract: Lanthanum strontium ferrite ($La_{0.85-x}Sr_{0.15}Ag_xFeO_{3-\delta}$ x = 0; LSFO) and its silver-doped derivative ($La_{0.85-x}Sr_{0.15}Ag_xFeO_{3-\delta}$ x = 0.05; LASFO) are synthesized using mild conditions by a sol−gel method. Both oxides present a perovskite-like structure with orthorhombic symmetry due to octahedral tilting; thus, the incorporation of silver in the A-site does not significantly modify the perovskite structure. Exsolution of silver nanoparticles (AgNPs) from LASFO is induced under mild conditions, resulting in Ag@LSFO samples[1]. X-ray absorption spectroscopy and synchrotron X-ray diffraction data reveal that the mechanism of exsolution involves the reduction of Ag^+ and the concomitant release of oxygen, without altering the oxidation state of Fe, inducing the formation of oxygen vacancies in the perovskite matrix. Homogeneous distribution of AgNPs on the perovskite matrix is observed by high-resolution transmission electron microscopy. The thermal evolution of Ag@LSFO proceeds through the progressive increase in oxygen vacancies that become thermally disordered. Subsequently, Ag nanoparticles were infiltrated into the porous, consolidated LSFO electrode (denoted as Ag_infil), and both the exsolved (Ag@LSFO) and infiltrated (Ag_infil) electrodes were subjected to electrochemical characterization. Their performance was evaluated and compared using electrochemical impedance spectroscopy (EIS).

Acknowledgment: *We thank "MCIN/AEI/10.13039/501100011033 and Fondo Europeo de Desarrollo Regional" (FEDER/UE "Una manera de hacer Europa") for funding the projects PID2022-139501OB-C21, PID2022-139501OB-C22, and PID2021-126323OA-I00. MTA, PRS, and UA also thank USP-CEU for financial support. We also thank the BM5 Spline line and CSIC for allocating beamtime and facilitate the access to ESRF for XAS experiments through grants A25-1044 and IH-MA-324.*

References

[1] J. Yu, L. Zhang *et al, Appl. Catal., B (2019), 256, No. 117818.*

Invited Talk-3

W2-I3. Environmental Assessment of MSW-to-FT Fuel Pathways: Impact of Gasification and Tail Gas Utilization Strategies

Jayakrishnan K. Ravindran[1,2*], Duncan P. Fagg[1,2], Margarida C. Coelho[2,3]
[1]*Department of Mechanical Engineering / Centre for Mechanical Technology and Automation (TEMA), University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro – Portugal*
[2]*LASI – Intelligent Systems Associate Laboratory, Guimarães, Portugal.*
[3]*Department of Environment and Planning / Centre for Mechanical Technology and Automation (TEMA), University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro – Portugal.*
[*]jayakrishnanravindran@ua.pt

Abstract:

The use of liquid fuels, especially in the transportation sector, is a significant contributor to climate change [1]. Another significant issue is that of municipal solid waste (MSW) disposal, with aprox 4 billion metric tonnes expected to be produced annualy by 2050 [2]. This study quantifies the environmental impacts associated with the production of drop-in fuels from MSW by combining gasification and the Fischer-Tropsch (FT) process. A cradle-to-gate life cycle assessment (LCA) compares four process configurations (direct or indirect gasification combined with a solid oxide electrolyzer (SOEC) or the water gas shift reaction (WGS) for H2/CO ratio correction) and two tail gas utilization strategies (recirculation within the system or combustion for energy generation) to identify the most environmentally friendly option. The functional unit of the study is 48.5 MJ of FT-fuel produced and the environmental impacts are quantified using the ReCiPe 2016 midpoint methodology on SimaPro 10.2.

Among the four process configurations, it is seen that combining direct gasification with an SOEC for H2/CO ratio correction leads to the lowest overall environmental impacts. Reductions of almost 20% can be seen in global warming potential (GWP) for this configuration as compared to direct gasification combined with WGS. The recirculation of tail gas with a recirculation ratio of 0.8 leads to a further reduction of global warming potential GWP by 42% as compared to energy generation with the tail gas. Similar trends are seen in all the other impact categories, with the most significant reductions seen in ozone formation potential (OFP) (51%) and fossil resource scarcity (FRS) (51%).

This study demonstrates that by using an SOEC and utilizing tail gas efficiently, significant reductions in environmental impacts can be achieved in drop-in fuel production from MSW.

Acknowledgment: *This abstract was supported by the projects UID 00481 Centre for Mechanical Technology and Automation (TEMA), 022.09319.PTDC, DOI 10.54499/2022.09319.PTDC, and COMPETE2030-FEDER-00770000 16527 2023.17134.ICDT. J.K. Ravindran thanks FCT for the Ph.D. scholarship 2023.02529.BD.*

References

[1] IPCC (2022), Emissions Trends and Drivers. In IPCC, 2022: Climate Change 2022: Mitigation of Climate Change. Contribution of Working Group III to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change. Cambridge University Press, Cambridge, UK and New York, NY, USA. doi: 10.1017/9781009157926.004.
[2] United Nations Environment Programme and International Solid Waste Association (2024), Global Waste Management Outlook 2024: Beyond an Age of Waste – Turning Rubbish into a Resource. United Nations Environment Programme, Nairobi, Kenya. Available at: https://wedocs.unep.org/20.500.11822/44939.

Invited Talk-4

W2-I4. Low-Temperature, Rapid Synthesis of Cu_3BiS_3 Thin Films for Sustainable Photovoltaics

C.O. Amorim[1*], M.S. Liborio[2,3], J.C.A. Queiroz[2], B.M.G. Melo[1], S.M. Sivasankar[1], T.H.C. Costa[2], M.P.F. Graça[1], and A.F. da Cunha[1]

[1] *Physics Department and i3N, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal*
[2] *Mechanical Engineering Department, Federal University of Rio Grande do Norte, University Campus, 59072-970 Natal, Brazil*
[3] *School of Science and Technology, Federal University of Rio Grande do Norte, University Campus, 59072-970 Natal, Brazil*
[*] amorim5@ua.pt

Abstract: The urgent demand for sustainable photovoltaic materials has driven research into alternatives to conventional absorbers like CIGS and CdTe, which rely on toxic or critical elements (In, Ga, Cd). Cu_3BiS_3 (CBS), a ternary chalcogenide, emerges as a promising candidate due to its optimal bandgap (≈1.34 eV), high absorption coefficient ($\alpha \geq 10^4$ cm^{-1}), and eco-friendly composition (Bi is abundant and nontoxic). However, most CBS synthesis methods require prolonged high-temperature sulfurization (>450 °C), hindering scalability and energy efficiency.

In this work, we demonstrate a rapid, low-energy route to phase-pure CBS films via Rapid Thermal Processing (RTP) sulfurization of e-beam evaporated Cu/Bi precursors.

By optimizing temperature (300–450 °C) and duration (2.5–15 min), we achieve high-quality CBS films at record-low conditions (350 ºC, 5 min), reducing considering the energy consumption when compared to conventional methods.

This approach balances crystallinity, phase purity, and optoelectronic performance, offering a scalable pathway for sustainable thin-film photovoltaics.

Acknowledgment: *This work is financed by national funds through FCT - Fundação para a Ciência e a Tecnologia, I.P. and the Ministry of Science, Technology and Higher Education under project LA/P/0037/2020, UIDB/50025/2020, UIDP/50025/2020*

References

[1] Libório, M. S., Queiroz, J. C. A. D., Sivasankar, S. M., Costa, T. H. D. C., Cunha, A. F. D., & Amorim, C. D. O. (2024). A review of Cu3BiS3 thin films: a sustainable and cost-effective photovoltaic material. Crystals, 14(6), 524.
[2] Amorim, C. O., Liborio, M. S., Queiroz, J. C. A., Melo, B. M. G., Sivasankar, S. M., Costa, T. H. C., Graça, P. M., & da Cunha, A. F. (2024). Cu3BiS3 film synthesis through rapid thermal processing sulfurization of electron beam evaporated precursors. Emergent Materials, 1-13.

4th International Workshop on Modern Trends in Energy Research
University of Aveiro, Portugal, 10 July, 2025

Invited Talk-5

W2-I5. Quantum-Informed Generative Optimization (QIGO) for Catalyst-Free Hydrogen Evolution Using Hybrid Quantum-AI

Jaykumar Lachure[1,2,*], **Sandhya K S**[2] , **Pukazhselvan D**[3], **Sagar Lachure**[4]

[1] KLEF Hydrabad, India
[2] Department of Chemistry, University of Kerala, Kariavattom, Thiruvananthapuram, 695581, Kerala, India
[3] Department of Mechanical Engineering, Centre for Mechanical Technology and Automation, University of Aveiro, 3810-193 Portugal
[4] Department of Computer Engineering & Information Technology, VJTI Mumbai 400019, India
Email: sagarlachure@gmail.com

Purpose: To address the growing global demand for sustainable hydrogen generation, we present a computational strategy for catalyst-free hydrogen evolution based on the Quantum-Informed Generative Optimization (QIGO) algorithm. This approach leverages advances in quantum confinement [1] and artificial intelligence [2,3] to propose optimized molecular candidates for efficient hydrogen evolution.

Methods: Quantum simulations were performed to determine the key electronic and reaction properties of water and hydrogen molecules, including ground-state energies and HOMO-LUMO gaps [1]. These quantum-derived features were input into a Machine Learning (ML) model trained with optimized hyperparameters to predict molecular efficiency. The feature space was informed by prior insights into machine learning for sustainable energy [4]. Statistical hypothesis tests (normality, ANOVA, t-tests) were employed to validate structure–performance relationships [5].

Results: Our best-performing ML model achieved a test R^2 of 0.432 and RMSE of 5.45. Feature importance analysis revealed that lipophilicity (logP) and dipole moment were the strongest predictors of efficiency [2]. The HOMO-LUMO gap was found to impact predicted performance significantly ($p < 0.001$), supporting previous findings on quantum-level effects in electrocatalysis [1,3]. The QIGO algorithm successfully generated five optimized molecules with predicted efficiencies above 78%.

Conclusion: This work demonstrates how combining quantum data with AI can lead to high-performing molecular candidates for catalyst-free hydrogen evolution—a promising pathway for scalable, clean energy production [1,4]. The QIGO framework offers a versatile and computationally affordable tool for rapid molecular discovery, aligning with the global shift toward digital-first, low-emission technologies [5].

References

[1] Zhou, Y., Zhang, X., Li, J., & Wang, H. (2024). *Quantum confinement-induced anti-electrooxidation for catalyst-free hydrogen evolution*. Nature Energy. https://doi.org/10.1038/s41560-024-01604-9
[2] Vipin, K. E., & Padhan, P. (2024). *Data-Driven Catalyst Design: A Machine Learning Approach to Predicting Electrocatalytic Performance in Hydrogen Evolution and Oxygen Evolution Reactions*. arXiv. https://doi.org/10.48550/arXiv.2412.12846
[3] Wayo, D. D. K., Chan, S. P., & Kim, T. Y. (2025). *AI and Quantum Computing in Binary Photocatalytic Hydrogen Production*. arXiv. https://doi.org/10.48550/arXiv.2501.00575
[4] Yao, Z., Kumar, P., & Fernandez, J. L. (2023). *Machine Learning for a Sustainable Energy Future*. Nature Reviews Materials. https://doi.org/10.1038/s41578-022-00490-5
[5] Frontiers in Materials. (2023). *Deep Generative Models for Materials Discovery and Machine Learning-Accelerated Innovation*. https://doi.org/10.3389/fmats.2022.865270

4th International Workshop on Modern Trends in Energy Research
University of Aveiro, Portugal, 10 July, 2025

Invited Talk-6

W2-I6. Improvement of cobalt-free perovskite electrodes for application in solid oxide fuel cells

Morena B. Farias[1,*], Allan J. M. Araújo[2,3], Laura I.V. Holz[2,3], Sergey M. Mikhalev[2,3], Rubens M. Nascimento[1], Carlos A. Paskocimas[1], Duncan P. Fagg[2,3], Francisco J.A. Loureiro[2,3]**
[1] *PPGCEM - Materials Science and Engineering Postgraduate Program, Federal University of Rio Grande do Norte – UFRN, Natal, 59078-970, Brazil*
[2] *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.*
[3] *LASI - Intelligent Systems Associate Laboratory, Portugal*
**morena.britof@gmail.com, **allan@ua.pt*

Abstract: Solid oxide fuel cells (SOFCs) are promising devices for efficient and clean energy generation. However, their performance is still limited by the oxygen electrode, i.e., the cathode[1]. In this study, we investigate the optimization of the $Sr_2Fe_{1.5}Mo_{0.5}O_{6-\delta}$ (SFM) oxygen electrode, a promising cobalt-free mixed ionic-electronic conduction material, and the SFM/CPO composite (fabricated with ~34 vol.% $Ce_{0.8}Pr_{0.2}O_{2-\delta}$ and featuring mixed conduction composite). We evaluate the effect of the microstructure and the impact of the number of layers of the electrode films deposited in electrolyte by analyzing the polarization resistance (R_{pol}) during the oxygen reduction reaction (ORR). In our electrochemical impedance spectroscopy (EIS) evaluation, both electrode materials produced showed a decrease in R_{pol} through successive deposited layers, in addition, the film thickness also helped in the electrochemical response through a higher solid fraction of material in the region close to the electrolyte[2,3]. However, the low electronic conductivity of CPO promoted a significant increase in the R_{pol} of the composite, despite the CPO improving the surface exchange kinetics[4]. Nevertheless, our research highlights microstructural and compositional criteria that are quite important for the development of research on new oxygen electrodes.

Acknowledgment: *The authors would like to acknowledge the following grants/projects: https://doi.org/10.54499/2020.02797.CEECIND/CP1589/CT0030, http://doi.org/10.54499/PTDC/CTM-CTM/2156/2020, COMPETE2030-FEDER-00770000, https://doi.org/10.54499/2022.09319.PTDC, https://doi.org/10.54499/2022.02498.PTDC, https://doi.org/10.54499/UIDB/00481/2020, 2023.05868.CEECIND https://doi.org/10.54499/2023.05868.CEECIND/CP2840/CT0021, https://doi.org/10.54499/UIDP/00481/2020, COMPETE2030 FEDER-00744500 of the Foundation for Science and Technology (FCT) and CENTRO-01-0145-FEDER-022083 of the Center of Portugal Regional Operational Program (Centro2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund (ERDF). This study was also funded in part by the Coordination for the Improvement of Higher Education Personnel - Brazil (CAPES) - Financial Code 001. Carlos A. Paskocimas thanks the National Council for Scientific and Technological Development (CNPq/Brazil, 302887/2022–9). Rubens M. Nascimento thanks the GRANT/CNPQ Project (314077/2020-0). The authors acknowledge the support provided by the National Agency of Petroleum, Natural Gas, and Biofuels (ANP) and the Human Resources Program (PRH), 2024/10542-0.*

References

[1] Farjana SH, Huda N, Mahmud MAP. J Sustain Min 2019;18:150-61.
[2] Araújo AJM, Loureiro FJA, Holz LIV, Grilo JPF, Macedo DA, Paskocimas CA, Fagg DP. Int J Hydrogen Energy 2021; 46:28258-69.
[3] Farias, MB, Araújo, AJ, Holz, LI, Mikhalev, SM, Paskocimas, CA, Fagg, DP, Loureiro, FJ. International Journal of Hydrogen Energy 2024; 61:1305-1316.
[4] Zapata-Ramírez V, Dos Santos-Gómez L, Mather GC, Marrero-López D, Pérez-Coll D. ACS Appl Mater Interfaces 2020; 12:10571–8.

Invited Talk-7

W2-I7. From Design to Performance: Redox-active COFs as advanced organic electrode materials

Raquel Dantas*[a], Olivera Lužanin[b,c], Maria Helena Braga[d,e], João Rocha[a] and Manuel Souto[a,f]

[a] *Department of Chemistry, CICECO-Aveiro Institute of Materials, University of Aveiro, Aveiro, 3810-393, Portugal*
[b] *National Institute of Chemistry, Hajdrihova 19, 1000, Ljubljana, Slovenia*
[c] *Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večnapot 113, 1000, Ljubljana, Slovenia*
[d] *Engineering Physics Department, Engineering Faculty, University of Porto, 4200-465, Porto, Portugal*
[e] *LAETA – INEGI, Institute of Science and Innovation in Mechanical and Industrial Engineering, 4200-465 Porto, Portugal*
[f] *CIQUS, Centro Singular de Investigación en Química Bioloxica e Materiais Moleculares, Departamento de Química-Física, Universidade de Santiago de Compostela, Santiago de Compostela, Spain*
e-mail: raqueldantas@ua.pt

In the pursuit of more sustainable and efficient energy storage technologies, redox-active Covalent Organic Frameworks (COFs) have emerged as a versatile class of organic electrode materials. Their structural tunability, porosity, and synthetic modularity allow for tailored electrochemical behavior across different battery chemistries. This work highlights how molecular design and system-level optimization can synergistically enhance the performance of COF-based electrodes for metal-ion batteries. [1].

This communication highlights how molecular design and system-level optimization can synergistically enhance the performance of COF-based electrodes. An anthraquinone-based n-type COF (DAAQ-TFP-COF) is used to study the influence of electrolyte and binder selection on performance. In lithium cells, four different electrolytes and two binders were tested, with the combination of LiTFSI in TEGDME and PTFE binder delivering the best performance and achieving near-theoretical specific capacities and high redox-site utilization. When applied in magnesium batteries, the same COF reveals electrolyte-dependent ion transport and reversibility, with chloride-free systems providing enhanced stability when compared to chloride-based electrodes. [2]. Recent studies have shown that the same COF can also operate effectively in aluminium using ionic liquid and deep eutectic solvents, delivering up to 113 mAh g^{-1} with 87% capacity retention over 400 cycles and Coulombic efficiencies above 95%. These findings demonstrate the feasibility of COFs in multivalent.

In parallel, a family of p-type tetrathiafulvalene (TTF)-based COFs was studied to explore structure-property relationships. Designed with varied linkers and tested in lithium half-cells, these materials exhibited high discharge potentials (~3.6 V vs. Li^+/Li), long-term cycling stability, and good rate capabilities. Their performance highlights the importance of electronic structure and framework architecture in accessing high-voltage organic cathodes. [3]

Overall, these results highlight that structural and molecular design, as well as electrolyte and binder optimization, are crucial in tuning COF's electrochemical performance and unlocking their full potential for various metal-ion battery systems.

References

[1] R. Dantas, C. Ribeiro, M. Souto, *Chem. Commun.* **2024**, 60, 138-149.

[2] O. Lužanin, R. Dantas, R. Dominko, J. Bitenc, M. Souto, *J. Mater. Chem. A*, **2023**, *11*, 21553-21560.

[3] G. Valente, R. Dantas, P. Ferreira, R. Grieco, N. Patil, A. Guillem-Navajas, D. Rodríguez-San Miguel, F. Zamora, R. Guntermann, T. Bein, J. Rocha, M.H. Braga, K. Strutyński, M. Melle-Franco, R. Marcilla, M. Souto, *J. Mater. Chem. A*, **2024**, 12, 24156-24164.

Acknowledgements: This work has received funding from the European Research Council (ERC) under the European Union's Horizon Europe Framework Programme (ERC-2021-Starting Grant, grant agreement no. 101039748-ELECTROCOFS). This work was developed within the scope of the project CICECO-Aveiro Institute of Materials, Grants UIDB/50011/2020 and UIDP/50011/2020, financed by national funds through the FCT/MEC and when appropriate co-financed by FEDER under the PT2020 Partnership Agreement. We thank FCT for funding the project PTDC/QUI-ELT/2593/2021. This study was also funded by the PRR─Plano de Recuperação e Resiliência and by the NextGenerationEU funds at the University of Aveiro through the scope of the Agenda for Business Innovation "New Generation Storage" (project no. 58 with the application C644936001–00000045).

4th International Workshop on Modern Trends in Energy Research
University of Aveiro, Portugal, 10 July, 2025

Invited Talk-8

W2-I8. Reactive Hydride Composites: A Promising Pathway for High-Capacity Hydrogen Storage

D. Pukazhselvan[1,2,*], **Duncan Paul Fagg**[1,2]

[1] *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.*
[2] *LASI - Intelligent Systems Associate Laboratory, 4800-058, Guimarães, Portugal.*
[*] dpukazh@ua.pt

Abstract:

Reactive Hydride Composites (RHCs) have emerged as a promising class of materials for solid-state hydrogen storage, with potential to reach the long-term hydrogen storage targets set by the U.S. Department of Energy (USDOE) [1]. By combining complex hydrides (e.g $LiBH_4$ and $Ca(BH_4)_2$) with selective binary metal hydrides (e.g MgH_2), RHCs enable coupled reactions that significantly improve the hydrogen storage behavior of the system kinetically and thermodynamically. For instance, $LiBH_4$ and $Ca(BH_4)_2$ are thermodynamically irreversible hydrides but their reaction with MgH_2 makes a reversible pathway as per the reactions (1) and (2),

$$2LiBH_4 + MgH_2 \rightarrow 2LiH + MgB_2 + 4H_2 \qquad (1)$$

$$Ca(BH_4)_2 + MgH_2 \rightarrow CaH_2 + MgB_2 + 4H_2 \qquad (2)$$

This synergistic approach facilitates hydrogen release at comparatively moderate temperatures with reversible capacities 11.4 wt.% and 8.3 wt.%, respectively, for (1) and (2). Nonetheless, despite the capacity advantages, challenges do remain, including high temperature/pressure operational requirements, slow kinetics and partial reversibility. Recent advances through approaches, such as nanoconfinement, catalytic modification, and ingredient substitution have shown promise in overcoming these limitations. For example, by incorporating a small quantity of TiB_2 in the RHS of the reaction (1) it is possible to improve reversibility and system kinetics and achieve consistent reversible behavior with capacity over 9 wt.%. Initial assessments reveal that TiB_2 does not participate in the RHC reaction path as a co-reactant but elevates the system behavior by playing the role of catalyst. Therefore, incorporation of a quantity as small as 0.05 molar ratio of TiB_2 is sufficient for improving the system dramatically. With such developments, RHC systems have become a candid class of reversible system for future hydrogen vehicles.

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

References

[1] USDOE, Target explanation document: onboard hydrogen storage for light-duty fuel cell vehicles, USDRIVE (2017), pp. 1-19.
[2] D. Pukazhselvan et al. Nanomaterials for Sustainable energy and environmental Remediation, Elsevier (2020), pp. 97-163.

Centre for Mechanical Technology Automation (TEMA),

Department of Mechanical Engineering, University of Aveiro

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

Today, TEMA addresses key global challenges faced by manufacturing and process industries, with a strong focus on automation, productivity, and optimisation. Recognising the dual importance of scientific impact and societal relevance, TEMA actively participates in international projects and networks, publishing widely in leading journals. While grounded in traditional mechanical engineering, the Centre continues to evolve into emerging fields such as nanotechnology, sustainable engineering, and artificial intelligence, ensuring a multidisciplinary and forward-looking research approach.

Mission

To create, implement, and disseminate scientific and technological knowledge that enables innovation and applied solutions in mechanical engineering and related areas—always in close collaboration with industry, and with a strong commitment to addressing the demands of a global society.

Vision

TEMA aspires to be at the forefront of technological progress, reinforcing its role as a multidisciplinary research unit. It promotes a global scientific culture, enhances the skills of future engineers and scientists, and fosters stronger research engagement within companies by encouraging the integration of doctoral-level researchers into the industrial sector.

Research

TEMA's research strategy is structured around three main mobilising programmes (MP):

- **MP1 – Sustainable Manufacturing Solutions**: Focused on developing and innovating manufacturing technologies to improve productivity, enhance quality, and reduce production waste.
- **MP2 – Techniques for Wellbeing**: Centred on engineering systems that improve quality of life by addressing human-centred needs.
- **MP3 – Research Infrastructure**: Dedicated to the strategic and efficient use of TEMA’s scientific equipment and human capital. The aim is to offer an open research infrastructure accessible to academia, research institutions, and industry.

TEMA is also a founding member of LASI – the Intelligent Systems Associate Laboratory, a consortium of 13 research units working together to drive innovation in intelligent systems (https://lasi-research.pt/).

In 2025, TEMA received the highest possible rating in the latest evaluation by the Portuguese Foundation for Science and Technology (FCT), earning an “Excellent” classification with full marks (15/15) across all evaluation criteria. TEMA was ranked first nationally among all mechanical engineering research units. This prestigious recognition highlights TEMA’s sustained commitment to research excellence, innovation, and collaboration. It also reflects the success of our multidisciplinary approach, the strength of our national and international partnerships, and the shared ambition of our team to lead and inspire in the fields of science and engineering.

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.

AGENDA ILLIANCE

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 CO_2 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/

AM2R - AGENDA MOBILIZADORA PARA A INOVAÇÃO EMPRESARIAL DO SETOR DAS DUAS RODAS

The Mobilizing Agenda for business innovation in the Two-Wheeled Sector aims to operationalize the intervention in priority areas in the value chain that will allow the transformation of the national production profile and the development of a new specialization profile in the sector to leverage its competitive position in the international market, focusing on independence from the Asian market, through the development and endogenization of advanced knowledge on new products, processes and services, increasing and differentiating national productivity and enhancing the dissemination of technological knowledge based on sustainability and digitalization. https://www.am2r.pt/

ATE - ALIANÇA PARA A TRANSIÇÃO ENERGÉTICA

The Alliance for Energy Transition aims to strengthen the competitiveness and resilience of companies in the energy sector as a result of the creation of innovative products and solutions of export nature, based on technology and know-how developed and consolidated in the sector, placing Portugal at the forefront of decarbonization and enabling an effective energy transition. The ATE will contribute significantly and sustainably to national strategic objectives, such as increasing exports, increasing investment in R&D, reducing CO_2 emissions, as well as changing the specialization profile of the economy. ATE Agenda

ILLIANCE
ENERGY EFFICIENCY

AM2R

PRR
Plano de Recuperação e Resiliência

REPÚBLICA
PORTUGUESA

Financiado pela
União Europeia
NextGenerationEU

Notes

Title
7th International Conference on
Nanomaterials Science and
Mechanical Engineering
Book of Abstracts

Editors
Igor Bdikin
Gil Alberto Batista Gonçalves
Martina Kocijan

Publisher
Universidade de Aveiro
1st edition – July 2025

ISBN
978-989-9253-17-9

tema university of aveiro
centre for mechanical technology and automation