tema university of aveiro
centre for mechanical technology and automation

International Conference on Nanotechnology Research and Innovation

November 20-24, 2023

University of Aveiro, Aveiro, Portugal

Book of Abstracts

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International Conference on Nanotechnology Research and Innovation, University of Aveiro, Portugal, November 20-24, 2023 (ICNTRI-2023)

ICNTRI-2023 looks for significant Modern Problems of Nanomaterials Research and Innovation, to provide a platform to the global researchers and practitioners from both academia as well as industry to meet and share cutting-edge development in the Nanotechnology science theories, modelling, experiments, industrial implementations.

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ICNTRI2023 program

November 20, 2023 (Monday)

1st International Workshop on “Modern Trends in Energy Research” Aveiro, Portugal, 20 November, 2023 **Auditorium 1**		Colloquium on Advances in materials for sustainability University of Aveiro, Portugal, 20 November, 2023 **Auditorium 2**		Workshop on High Valued Developments in Photocatalysis Haribhai V. Desai Arts, Science & Commerce College, Pune, India, 20 November, 2023 **Auditorium 3**	
9.20 - 9:30	**WELCOME ADDRESS** Dr. Pukazh Selvan Dharmakkon	**9.20 - 9:30**	**WELCOME ADDRESS** Dr. Eskilla Venkata Ramana and Dr. Indrani Coondoo		
09:30 – 10:00	***Plenary Lecture*** **Prof. Dr. Gunnar Suchaneck** *TU Dresden, Solid-State Electronics Laboratory, 01062 Dresden, Germany.* Title: **Solid oxide fuel cells based on nonstoichiometric strontium ferromolybdate electrodes**	**09:30 – 10:30**	**Dr Jiri Rathorsky (Invited)** *J. Heyrovský institute of physical chemistry of the CAS, Prague, Czech Republic* **Photocatalytic degradation of aqueous pollutants**	**9:40 - 10:00**	**WELCOME ADDRESS** Dr. Vikram U. Pandit, Dr. Rajendra G. Gurao
10:00 – 10:20	**W1-O1** **Allan J. M. Araúj** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal* Title: **Transition metal carbides as potential anode components for Proton Ceramic Fuel Cells (PCFCs)**			**10:00 - 10:30**	***W2-IT1*** **Prof. Ganesh Jadhav** *Haribhai V. Desai College, Pune, India* **Water Purification using Ex-situ Catalyst system**
10:20 – 10:35	**W1-O2** **Alfredo S. B. Luemba** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal* **Title: Synthesis of carbon and sulfur-resistant electrolytes for proton ceramic membrane reactors**				
10:35 – 10:50	**W1-O3** **E. Durana** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal* **Title: Reversible electrodialysis: a salinity gradient power source**	**10:30 – 11:15**	**Dr Xiao Long (Invited)** *Institute of Microelectronics, Chinese Academy of Sciences, Beijing, China* **Non-volatile optically controlled BTO ferroelectric tunnel junctions and CMOS compatible volatile HZO ferroelectric tunnel junctions**	**10:30 - 11:00**	***W2-IT2*** **Prof. Vivekanand Jawale** *RKM College, Akurdi, Pune, Maharashtra 411035, India* **Dye Degradation using Organic Inorganic Catalyst**

10:50 – 11:05	**W1-O4** **Ihsan Çaha** *International Iberian Nanotechnology Laboratory, Avenida Mestre José Veiga s/n, 4715-330 Braga, Portugal* **Title: Chemical bath deposition of Zn1-xSnxOy thin films and their application as buffer layers for Cd-free Cu(In, Ga)Se2 solar cells**				
11:05 – 11:20	**W1-O5** **Catarina de Lemos** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal* **Title: Study of rGO-MIL101(Cr) as the anode of a half-cell**			11:00 - 11:30	***W2-IT3*** **Dr. Sachin Wadhai** *Savitribai Phule Pune University, Pune, India* **Water Splitting**
11:20 – 11:30	**Coffee break / Open discussions**	11:15 – 12:00	**Dr V Raghavendra Reddy (Invited)** *UGC-DAE, Indore, India* **Magnetism in ferroelectric four-layered Aurivillius $Bi_5FeTi_3O_{15}$ compound**		
11:30 – 11:50	**W1-O6** **Dr. Francisco J. A. Loureiro** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal* **Title: TiO2/MgH2-based anodes for lithium-ion batteries**			11:30 - 12:00	***W2-IT4*** **Prof. Omkar Malusare** *H. V. Desai College, Pune India* **Water Purification using In-situ Catalyst system**
11:50 – 12:05	**W1-O7** **Thayse R. Silva** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal* **Title: Compositional optimization of MnCo2O4@rGO electrocatalysts for oxygen evolution reaction**				
12:05 – 12:25	**W1-O8** **Dr. Laura I. V. Holz** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal* **Title: Exploring Vanadium (Oxy)nitride as a Promising Anode Material for Ammonia Solid Oxide Fuel Cells**	12:00 – 12:20	**Daniela Santos (Oral)** *Universidade do Minho, Braga, Portugal* **Functionalized Nanofibers with Cyclodipeptides for Thermal Sensing and Energy Harvesting**	12:00 - 12:40	**PP1: Bhagwan Daphal** **PP2: Jatin Mithari** **PP3: Ganesh Dawange** **PP4: Purnima Patil**

12:25 – 12:45	**W1-O9** **Paula Rosendo Santos** *Universidad San Pablo-CEU, Facultad de Farmacia, Departamento de Química y Bioquímica, Urbanización Montepríncipe, Boadilla del Monte, E-28668, Madrid, Spain* **Title: Optimization of the electrochemical performance of Nd1/3Sr2/3CoO3−δ cathode for solid oxide fuel cells via spray-pyrolysis deposition and decoration with Ag nanoparticles**	12:20 – 12:40	**Bruna M. Silva (Oral)** *Universidade do Minho, Braga, Portugal* **Strain dependent magnetic and dielectric properties of Ca3Mn2O7 thin films prepared by pulsed laser deposition**		
12:45 – 13:00	**W1-O10** **Dr. D. Pukazhselvan** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal* **Title: Comments on the suitable hydrogen storage materials for vehicular applications**	12:40 – 13:00	**Vishakha Sharma (Oral)** *DTU, India* **Metalens Magic-Shaping the Future of nanostructure probing**	12:40 - 13:00	**Final discussions and comments**
12:30 – 14:00	Lunch break	13:00 - 14:30	Lunch break	13:00 - 14:30	Lunch break
Workshop on New Challenges of Bionanomaterials: Science, Technology, Application University of Aveiro, Portugal, 20 November, 2023 **Auditorium 1**		**Colloquium on Advances in materials for sustainability University of Aveiro, Portugal, 20 November, 2023** **Auditorium 2**			
14.00 - 14:20	**WELCOME ADDRESS** Dr. Igor Bdikin, Dr. Alejandro Heredia Barbero				
14:20 - 14:50	Chair: Dr. Gil Gonçalves ***Invited talk W3-I1*** **Levodopa-Functionalized Gold Nanourchins as Highly Efficient Nanosensors for Detecting Contaminants** Prof. Dr. Ricardo João Borges Pinto *Department of Chemistry, University of Aveiro, Portugal*	14:30 – 15:15	**Dr Buchi Suresh (Invited)** *International advanced research centre for powder metallurgy (ARCI), Hyderabad, India* **Solid Oxide Cells (SOFC/SOEC): An energy efficient clean and green technology for the production of energy and hydrogen**		

14:50 - 15:10	***W3-O1*** **Gold nanoparticles (Eco)toxicity** Valérie Carvalho *Department of Biology, University of Aveiro, Portugal*				
15:10 - 15:30	***W3-O2*** **Comparative assessment of the cytotoxicity of fuel- and bio-based micro(nano)plastics: amphibian cells as biological models** Carolina Frazão *Department of Biology, University of Aveiro. Portugal*	**15:15 – 15:35**	**Dr. V.C. Bharath Sabarish (oral)** *K. Ramakrishnan College of Technology, Trichy, India* **Effect of particles/ions irradiation on Triglycine sulphate single crystal on its ferroelectric and piezoelectric properties**		
15:30 – 15:40	**Coffee break / Open discussions**	**15:35 – 16:20**	**Dr. Dhiren K Pradhan (Invited)** *University of Tennessee and Oak Ridge National Laboratory, USA* **Ferroelectric / Multiferroic Materials for Non-Volatile memory Applications**		
15:40 - 16:00	***W3-O3*** **Bovine Serum Albumin Nanoparticles as Drug Delivery Systems for Prostate Cancer Treatment** Dr. Beatriz Teixeira *Department of Biology, University of Aveiro, Portugal*				
16:00 - 16:50	***W3-O4*** **Atomic force microscopy of organic microstructures** Dr. Igor Bdikin *Department of Mechanical Engineering, University of Aveiro*	**16:20 - 16:30**	**Final discussions and comments**		
16:50 - 17:00	**Final discussion and comments**				

November 21, 2023 (Tuesday)

International Conference on Nanotechnology Research and Innovation (ICNTRI-2023) (*online*)	
9:00-9:30	**Auditorium 1** **WELCOME ADDRESS**: Dr. Igor Bdikin, Prof. Dr. Vikram Uttam Pandit, Prof. Dr. Gunnar Suchaneck, Prof. Dr. Heberton Wender, Dr. Gil Alberto Batista Gonçalves
9:30-10:20	Session: Smart and multifunctional materials CHAIR: Dr. Gonzalo Guillermo Otero Irurueta ***Plenary Lecture*** Prof. Dr. Pedro Martins **Magnetoactive (multi)functional materials by additive manufacturing** *BCMaterials, Parque Científico y Tecnológico de Bizkaia, Derio, Spain / IKERBASQUE, Basque Foundation for Science, Bilbao, Spain*
10:20-10:30	Coffee break
10:30-11:30	Session: New Energy Materials CHAIR: Dr. Gonzalo Guillermo Otero Irurueta ***Plenary Lecture*** Prof. Dr. Nikolai Sobolev **Energy, demand for computing power and the Green World** *i3N and Departamento de Física, Universidade de Aveiro, 3810-193 Aveiro, Portugal*
11:30-12:30	Session: New Energy Materials ***Plenary Lecture*** Prof. Dr. Binay Kumar **Nanoparticle based piezoelectric energy harvesters** *Crystal Lab, Department of Physics & Astrophysics, University of Delhi, India*
12:30-13:00	Session: Rare earth thermometry ***Keynote talk*** Dr. Pavani Krishnapuram **(I29)** **Analogy of different optical temperature sensing techniques in rare earth doped materials** *I3N-Department of Physics, University of Aveiro, Aveiro, Portugal*
13:00-13:30	Lunch

13:30- 14:30	Session: Nanotechnology CHAIR: Dr. Gil Gonçalves ***Plenary Lecture*** Prof. Dr. Ajeet Kaushik **Can nanotechnology for tackle state-of-the-art issues?** *Florida State University, USA*
14:30- 15:20	Session: Nanotechnology ***Plenary Lecture*** Prof. Dr. Jose Angel Martín Gago **Mimicking cosmic-dust formation: exotic nanoparticles and vacuum technology** *Institute of Material Science of Madrid-CSIC, Spain*
15:20- 15:35	Coffee break
15:35- 16:15	Session: Micro / Nano Materials CHAIR: Dr. Gil Gonçalves ***Keynote talk*** Dr. Alejandro Heredia Barbero **(I9)** **Nanotechnological Methods to Characterize the Allende Meteorite** *Departamento de Química de Radiaciones y Radioquímica, Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, Mexico*
16:15- 16:45	Session: Biomaterials ***Keynote talk*** Prof. Dr. Cicero R. Cena **(I28)** **Improving sample classification for photodiagnosis** *Instituto de Física, UFMS – Mato Grosso do Sul Federal University, Brazil*
16:45- 17:00	Session: Biomaterials Bartosz Klębowski **(O30)** **The influence of ultrasmall palladium nanoparticles (Pd NPs) PEGylation on their radiosensitizing effect in simulated proton radiotherapy of glioblastoma multiforme (in vitro model)** *Institute of Nuclear Physics Polish Academy of Sciences, 30-342 Kraków, Poland*
17:00- 17:30	Session: Biomaterials ***Keynote talk*** Dr. Pankaj Bharmoria **(I3)** **Photochemistry of Triplet-State and Exploitation in Solid-state Photo-switching** *The Institute of Materials Science of Barcelona, ICMAB-CSIC, Bellaterra, 08193 Barcelona, Spain*

17:30- 18:00	Session: Nanotechnology *Keynote talk* Dr. E.Venkata Ramana **(I24)** **Dimensionally modified structures for caloric applications: an experimental study** *I3N, Department of Physics, University of Aveiro, Aveiro 3810-193, Portugal*
18:00- 18:15	Session: Biomaterials Zinaida Shakel **(O26)** **Comparative analysis of kappa- and iota-carrageenan hydrogels for effective skin delivery** *LAQV, REQUIMTE, Department of Chemistry, Faculty of Pharmacy, University of Porto, R. Jorge de Viterbo Ferreira 228, 4050-313 Porto, Portugal*
18:15- 18:30	Session: Composites Dr. Martina Kocijan **(O43)** **Degradation of methylene blue using TiO2/reduced graphene oxide nanocomposite by advanced oxidation process** *Department of Materials, Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Ivana Lučića 5, 10000 Zagreb, Croatia*

November 22, 2023 (Wednesday)

International Conference on Nanotechnology Research and Innovation (ICNTRI-2023) (*online*)	
8:30- 8:45	Session: Nanocomposites CHAIR: Prof. Dr. Neeraj Panwar Nahid Tyagi **(O45)** **Novel S-scheme based nanocomposite of MXene/V2O5 for photocatalytic degradation of Crystal Violet from Contaminated water** *Department of Physics and Astrophysics, Central University of Haryana, Mahendragarh-123031, India*
8:45- 9:00	Session: New Energy Materials Robin Saini **(O46)** **A synergistic composite of rGO/MOF-5 for Electrochemical Energy Storage** *Department of Physics and Astrophysics, Central University of Haryana, Haryana, Mahendergarh, India*
9:00- 9:15	Session: Electrical Measurements and Instrumentation Jyoti Chauhan **(O42)** **Analysis and measurements of the properties of light through Photonic crystal Fibers** *TIFAC-Center of Relevance and Excellence in Fiber Optics and Optical Communications, Department of Applied Physics, Delhi Technological University, Bawana Road, Delhi 110042, India*
9:15- 9:45	Session: Ceramics ***Keynote talk*** Dr. Oleksandr Tkach **(I26)** **Behind the enhanced electrical performance of Flash sintered potassium sodium niobate ceramics** *Department of Materials and Ceramic Engineering, CICECO – Aveiro Institute of Materials, University of Aveiro, Aveiro 3810-193, Portugal*
9:45- 10:30	Session: Materials Science ***Plenary Lecture*** Prof. Dr. Yulian Vysochanskii **Formation of multipolar states in layered $CuInP_2S_6$ ferrielectrics** *Institute for Solid State Physics and Chemistry, Uzhhorod University, Uzhhorod 88000, Ukraine*
10:30- 10:40	Coffee break

10:40- 11:20	Session: Nanofluids CHAIR: Prof. Dr. Neeraj Panwar ***Keynote talk*** Prof. Dr. Mónica Sandra Abrantes de Oliveira Correia **(I13)** **Nanofluids for heat transfer enhancement: challenges and opportunities** *Centre for Mechanical Technology and Automation (TEMA), Department of Mechanical Engineering, University of Aveiro, Campus Universitário de Santiago, 3810 - 193 Aveiro, Portugal; LASI—Intelligent Systems Associate Laboratory,4800-058 Guimarães, Portugal*
11:20- 11:50	Session: Nanotechnology ***Plenary Lecture*** Prof. Dr. Salam J.J. Titinchi **Functionalized PEI Coated Magnetic Nanoparticle Sorbents for Removal of Lead from Aqueous Solution** *Department of Chemistry, University of the Western Cape, Cape Town, South Africa*
11:50- 12:20	Session: Biomaterials ***Keynote talk*** Prof. Dr. Serbülent Türk **(I18)** **Nanofiber-Based Hydrogels for Drug Delivery Systems** *Sakarya University, Biomedical, Magnetic and Semiconductor Materials Application and Research Center (BIMAS-RC), 54187 Sakarya, Turkey*
12:20- 12:35	Session: Biomaterials Ş. Balcı **(O9)** **Contact angle and surface energy behavior of poly (vinyl alcohol)/ poly (ethylene glycol)/carbon nanotube/doxorubicin hybrid hydrogels** *Sakarya University, Biomedical Engineering, Institute of Natural Sciences, Esentepe Campus, 54187 Sakarya, Turkey*
12:35- 12:50	Session: Biomaterials Engin GEPEK **(O10)** **Ink Preparation for Supportless 3D Printing Of PVA/ALG/HA Composite Scaffolds** *Sakarya University, Mechanical Engineering Department, Sakarya-Turkey*
12:50- 13:05	Session: Biomaterials Turan İbrahimova **(O17)** **Artificial Knee Implant Design and Analysis with Finite Element Method** *Sakarya University, Mechanical Engineering Department, Sakarya-Turkey*
13:05- 13:20	Session: Journal presentations Nevena Lukic **(J1)** **Journal Applied Sciences** *MDPI AG, St. Alban-Anlage 66, 4052 Basel, Switzerland*

13:20-14:00	Lunch
14:00-14:30	Session: Nanotechnology: Coatings, Organic films CHAIR: Dr. D. Pukazhselvan ***Plenary Lecture*** Prof. Dr. Vincent Ball **Electrodeposition of polyphenols and of nitrogen containing polyphenols** *Université de Strasbourg. Faculté de Chirurgie Dentaire. 8 rue Sainte Elizabeth. 67000 Strasbourg, France*
14:30-15:00	Session: Biomaterials ***Keynote talk*** Dr. Gil Gonçalves **(I10)** **Graphene-based nanocomposites for environmental and health applications** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal*
15:00-15:15	Session: Biomaterials Yağmur Camcı **(O20)** **Synthesis, Water Retention Capacity and Swelling Behavior of Polyvinyl Alcohol/Carboxymethyl Cellulose Hydrogels Mimicking Dermis and Epidermis** *Sakarya University, Institute of Natural Sciences, Biomedical Engineering, Esentepe Campus, 54187, Sakarya, Turkiye*
15:15-15:30	Session: Biomaterials Shaimaa Obaid Hasson **(O11)** **Anti-genic Effect of Green Synthesized Zinc Oxide Nanoparticles on Biofilm Gene Expression in MDR uropathogenic E.coli** *Department of Biotechnology, College of Biotechnology, Al-Qasim Green University, Al-Qasim, Iraq*
15:30-15:45	Session: Metal alloy Materials Prof. Dr. Mehmet İskender ÖZSOY **(O18)** **Surface characterization of CNT coated aluminum alloy** *BIOE ℕAMS, (Biomaterials, Energy, Photocatalysis, Enzyme Technology, Nano and Advanced Materials, Additive Manufacturing, Environmental Applications and Sustainability Research and Development group), Sakarya University, Sakarya, Turkey*
15:45-16:00	Coffee break
16:00-16:30	Session: Coatings CHAIR: Dr. D. Pukazhselvan ***Keynote talk*** Dr. Ana Violeta Girão **(I27)** **Towards Chromium (VI) Replacement: Combination of Electrochemical Deposition and PVD Coatings** *CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Aveiro, 3810-193, Portugal*

16:30-17:00	Session: Multifunctional materials ***Keynote talk*** Prof. Dr. Vikram Uttam Pandit **(I6)** **Water Pollution Control and Hydrogen production using Multifunctional Organic & Inorganic Photocatalyst** *Haribhai V. Desai Arts, Science & Commerce College, Pune-411002, India*
17:00-17:15	Session: Metal alloy Materials Wasan A. Alkaron **(O40)** **The effects of black tea extracts on the corrosion inhibition of mild steel in acidic solution** *Technical Institute of Basra, Southern Technical University, Basra, Iraq*
17:15-17:30	Session: Metal alloy Materials Dr. Oksana Bersirova **(O32)** **Electrolytic rhenium alloys with iron-group metals: synthesis, properties and applications** *Department of Physical Chemistry, Vilnius University, Vilnius, Lithuania*
17:30-18:00	Session: Micro / Nano Materials ***Keynote talk*** Dr. César Martínez-Flores **(I22)** **Analogous environment study of the Naica mine (dehydrated calcium sulfate CaSO4·2H2O): A DFT approach to molecular dynamics** *Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, Circuito Exterior C.U., Ciudad de México, 04150, México*
18:00-18:15	Session: Protective Coatings and Corrosion of Materials Amira Gharbi **(O12)** **Corrosion assessment of nickel electrowinning coatings from watts bath in 0.5N NaCl** *Process Engineering Department, Physics of Matter and Radiation Laboratory LPMR, Mohamed Chérif Messaadia university, Souk Ahras 41000 Algeria*
18:15-18:30	Session: Micro / Nano Materials Dr. Igor Bdikin **(O33)** **Local properties of mild steel** *TEMA: Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal*
18:30-18:45	Session: Nanocomposites Dr. Omkar Malusare **(O47)** **Ex-Situ synthesis of Fe_2O_3-TiO_2 nanocomposites for photocatalytic applications** *Haribhai V. Desai College of Commerce, Arts and Science, Pune-411002, India*
18:45-19:15	CHAIR: Dr. D. Pukazhselvan **Evening Poster Session** **P1-P6**

November 23, 2023 (Thursday)

International Conference on Nanotechnology Research and Innovation (ICNTRI-2023) (*online*)	
9:00-9:30	Session: Engineering & Technology CHAIR: Dr. Indrani Coondoo ***Keynote talk*** Prof. Dr. Henrikas Cesiulis **(I25)** **Innovation in Chemical and Electrochemical Treatment and Recovery of Precious Metals** *Vilnius University / EPT , Lithuania*
9:30-10:00	Session: Protective Coatings and Corrosion of Materials ***Keynote talk*** Prof. Dr. Natalia Tsyntsaru **(I15)** **Composite/hybrid coatings as an innovative way to improve electrodeposited materials** *AInstitute of Applied Physics, Moldova State University, MD-2028 Chisinau, Moldova*
10:00-10:30	Session: Thin Films ***Keynote talk*** Dr. Joana Catarina Mendes **(I2)** **Improving the thermal management of electronic devices with diamond films** *Instituto de Telecomunicações e Departamento de Eletrónica, Telecomunicações e Informática, Universidade de Aveiro, Portugal*
10:30-11:00	Session: Thin Films ***Keynote talk*** Dr. Svitlana Kopyl **(I17)** **Development of biocompatible thin piezoelectric films for various applications** *CICECO-Aveiro Institute of Materials, Physics Department, University of Aveiro*
11:00-11:15	Coffee break
11:15-11:45	Session: Thin Films CHAIR: Dr. Indrani Coondoo ***Keynote talk*** Dr. Fábio G. Figueiras **(I14)** **Growth and structural characterization of h-LuMnO3 thin films deposited by MOCVD** *IFIMUP & Department of Physics and Astronomy, Sciences Faculty, University of Porto, R. Campo Alegre 687, 4169-007 Porto, Portugal*

11:45- 12:15	Session: Magnetic Materials ***Plenary Lecture*** Prof. Dr. Gunnar Suchaneck **Perspectives of strontium ferromolybdate-based magnetic tunnel junctions** *TU Dresden, Solid-State Electronics Laboratory, 01062 Dresden, Germany*
12:15- 12:45	Session: Composites ***Keynote talk*** Prof. Dr. Neeraj Panwar **(I21)** **Photocatalytic performance of Rare-earth orthchromite-reduced graphene oxide nanocomposites for wastewater treatment** *Department of Physics, Central University of Rajasthan, Bandarsindri-305817, Rajasthan, India*
12:45- 13:15	Session: Composites ***Keynote talk*** Prof. Dr. Radheshyam Rai **(I5)** **Impedance modulated dielectric and magneto dielectric properties of Lead free KNN and NiTiO3 based composite ceramics** *Eternal Univ, Dept Phys, Akal Coll Basic Sci, Sirmour, Himachal Prades, India*
13:15- 14:00	Lunch
14:00- 14:30	Session: Optical/Electronic/Magnetic Materials CHAIRs: Dr. Francisco Loureiro and Dr. Alejandro Heredia Barbero ***Keynote talk*** Dr. Suresh Kumar Jakka **(I11)** **Enhancing Light Efficiency for Horticulture with Rare-Earth and Transition Metal-Doped Phosphors** *I3N & Physics Department, University of Aveiro, Aveiro 3810-193, Portugal*
14:30- 15:00	Session: Optical/Electronic/Magnetic Materials ***Keynote talk*** Dr. M. Jayasimhadri **(I12)** **Structural and photoluminescence studies rare earth doped metasilicate phosphor for solid state lighting applications** *Luminescent Materials Research Lab, Department of Applied Physics, Delhi Technological University, India*
15:00- 15:15	Session: New Energy Materials Y.M.I.B. Samarakoon **(O19)** **Understanding the effect of fluoroethylene carbonate addition into an electrolyte - a molecular dynamics study** *National Center for Advanced Battery Research, National Institute of Fundamental Studies, Hantana Road, Kandy, Sri Lanka*

15:15- 15:30	Session: New Energy Materials KAHNU CHARAN PRADHAN **(O3)** **Cyclometallated Iridium Complexes containing ppy type ligands** *Department of Chemistry, Utkal University, Bhubaneswar, Odisha, India*
15:30- 15:45	Session: New Energy Materials W. T. R. S. Fernando **(O15)** **Electrochemical performance of Cu2O anode material synthesized by electrodeposition method for rechargeable lithium-ion batteries** *National Center for Advanced Battery Research, National Institute of Fundamental Studies, Sri Lanka*
15:45- 16:00	Coffee break
16:00- 16:30	Session: New Energy Materials CHAIRs: Dr. Francisco Loureiro and Dr. Alejandro Heredia Barbero ***Keynote talk*** Prof. Dr. Cauê Alves Martins **(I16)** **Paper-based microfluidic fuel cells fed by eco-friendly organics** *Institute of Physics, Federal University of Mato Grosso do Sul, Brazil*
16:30- 17:00	Session: Materials under Irradiation ***Plenary Lecture*** Prof. Dr. Ezddin Hutli **Evaluation of Materials Characteristics Acting as a Carrier for Boron Compounds During Neutron Irradiation and Study of Relevant Boron Compounds (H3BO3, B-DTPA) Usually Employed in BNCT-Technique under Neutron Irradiation in a Medically Relevant Reactor Neutron Source** *Centre for Energy Research, Budapest, Hungary*
17:00- 17:15	Session: New Energy Materials Prof. Dr. Soner ÇAKAR **(O5)** **Investigation and effect of CeVO4/TiO2/SnS composite on synthesis and oxygen evaluation reactions (OER)** *Zonguldak Bülent Ecevit University, Faculty of Science, Department of Chemistry, 67100 Zonguldak, Turkey*
17:15- 17:30	Session: New Energy Materials Dr. Ramunas Levinas **(O31)** **Plasma electrolytic oxidation synthesis of TiO2/CuO heterostructures and characterization for photoanode applications** *Center for Physical Sciences and Technology (FTMC), Saulėtekio ave. 3, Vilnius, Lithuania*
17:30- 17:45	Session: Hydrogen and Fuel Cell Science Allan J. M. Araújo **(O34)** **Revealing surface exchange kinetics on the new layered barium cobaltite electrode for Protonic Ceramic Cells (PCCs)** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal*

17:45- 18:00	Session: New Energy Materials Maria B. Candeias **(O39)** **Perovskite thin films: Optoeletronic properties** *Departamento de Física and I3N, Universidade de Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal.Centre for Mechanical Technology and Automation, Mechanical Engineering Department, University of Aveiro, Aveiro, 3810-193, Portugal*
18:00- 18:15	Session: Hydrogen and Fuel Cell Science Aleksandr Bamburov **(O27)** **Selecting a buffer layer for high-temperature carbon-assisted electrolysis cell with SrFe0.75Mo0.25O3-δ anode** *CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal*
18:15- 18:30	Session: Hydrogen and Fuel Cell Science Rui Pinto **(O28)** **Characterization of CaVO3, SrVO3 and SrMoO3 perovskites as anode materials for biogas-fueled solid oxide fuel cells** *CICECO – Aveiro Institute of Materials, University of Aveiro, Aveiro, Portugal*
18:30- 18:45	Session: Hydrogen and Fuel Cell Science Dr. Laura I. V. Holz **(O29)** **Exploring Yttrium-Doped Zirconate Stannate (BaZr0.8-xSnxY0.2O3-□) proton-conducting electrolytes: Synthesis, characterization, and stability in CO2 environment** *Centre for Mechanical Technology and Automation, Mechanical Engineering Department, University of Aveiro, Aveiro, 3810-193, Portugal*

November 24, 2023 (Friday)

International Conference on Nanotechnology Research and Innovation (ICNTRI-2023) (*online*)

8:45- 9:00	Session: Nanostructures and applications CHAIRs: Dr. Suresh Kumar Jakka and Dr. Milan Vukšić Prof. Dr. Fehim Findik **(O49)** **Nanostructures and applications** *Metallurgy and Materials Engineering Department, Faculty of Technology, Sakarya University of Applied Sciences, Sakarya, Turkey*
9:00- 9:15	Session: Micro / Nano Materials Prof. Dr. Jamal Davoodi **(O2)** **Investigation of mechanical properties in new 2D-structure Irida-Graphene by using molecular dynamics simulation** *Faculty of science, University of zanjan, Zanjan, Iran*
9:15- 9:30	Session: Micro / Nano Materials Prof. Dr. Muhammad Ajmal **(O23)** **Fabrication of dual responsive polymer microgel containing silver nanoparticles with catalytic and antibacterial activity** *Department of Chemistry, Division of Science and Technology, University of Education, Lahore, Pakistan*
9:30- 9:45	Session: New Materials and Advanced Materials H.M.H.D.K. Naranpanawa **(O16)** **Developing Vein Graphite Anode Materials for Li-ion Batteries by Optimizing and Scaling up of Chemically Mild Oxidation** *National Center for Advanced Battery Research, National Institute of Fundamental Studies, Kandy, Sri Lanka*
9:45- 10:15	Session: Micro / Nano Materials ***Keynote talk*** Prof. Dr. S. Shanmuga Sundari **(I7)** **Effect of swift heavy ion irradiation on lithium borate glasses** *Department of Physics, Seethalakshmi Ramaswami College, Trichy, 620002, India*
10:15- 10:30	Session: Low Dimension Structures Justyna Niewiadomska-Kaplar **(O22)** **Atomic system: the structuring mechanisms of atomic shells** *Scientific Publishing House Tab, Viale Manzoni 24c, 00185, Rome, Italy*
10:30- 10:45	Coffee break

10:45-11:15	Session: Nanotechnology CHAIRs: Dr. Suresh Kumar Jakka and Dr. Milan Vukšić ***Keynote talk*** Prof. Dr. Musaab ZAROG **(I4)** **Piezoelectric nanogenrators for self-powered Internet-of-Things (IoT) devices** *Sultan Qaboos University, Oman*
11:15-11:30	Session: Nanotechnology Dr. Vivekanand Jawale **(O48)** **Synthesis of organic-inorganic semiconductor photocatalysts and their composites for environmental remediation** *Department of Chemistry Modern College of Engineering, Shivajinagar, Pune-411005, India*
11:30-12:00	Session: Nanotechnology ***Keynote talk*** Prof. Dr. Allisson Saiter-Fourcin **(I23)** **Contribution of nanoscale calorimetry to material characterization** *Univ Rouen Normandie, INSA Rouen Normandie, CNRS, Groupe de Physique des Matériaux UMR 6634, F-76000 Rouen, France*
12:00-12:15	Session: Nanotechnology Melike Akarsu **(O21)** **Doping of TiO2 with different metals to enhance the performance of dye-sensitized solar cells** *Sakarya University, Institute of Natural Sciences, Department of Chemistry, 54187, Sakarya, Turkiye*
12:15-12:30	Session: New Materials and Advanced Materials R. El Otmani **(O24)** **Effect of Thiourea Concentration on Physical Properties of Sprayed Cu2MnSnS4 Thin Films** *LNMAMT, Université Hassan II, Faculté des Sciences et Techniques, BP 145 Mohammedia Morocco*
12:45-13:00	Session: Probing techniques in nanostructures Vishakha Sharma **(O41)** **Metalens Magic-Shaping the Future of Nanostructure Probing** *TIFAC-Center of Relevance and Excellence in Fiber Optics and Optical Communication, Department of Applied Physics, Delhi Technological University, Delhi, India*
13:00-13:15	Session: Stimuli Responsive Biomaterials Mahsa Heidarnejad **(O14)** **Synthesis of Fe3O4 magnetic nanoparticles, modifying with tannic acid and loading and releasing application of salicylic acid** *Sakarya University, Faculty of Science, Department of Chemistry, 54050 Sakarya, Turkiye*
13:15-14:00	Lunch

14:15- 14:30	Session: Nanotechnology CHAIRs: Dr. Laura Holz and Dr. Martina Kocijan ***Keynote talk*** Prof. Dr. Alaa Almansoori **(I8)** **A new approach to key challenges in additive manufacturing by laser sintering** *Southern Technical University, Basra, Iraq*
14:30- 14:45	Session: New Materials and Advanced Materials Burak ÜNLÜ **(O8)** **Fabrication of Novel Gellan Gum or Polyvinylidene Fluoride Based Gels Containing LiTFSI, Self-Polymerized PEDOT and I-/I3- Redox Couple** *Sakarya University, Biomedical, Magnetic and Semiconductor Materials Research Center (BIMAS-RC), 54187, Sakarya, Turkey*
14:45- 15:00	Session: Sensor Materials Esra KALEOĞLU **(O6)** **The ITO/rGO@SnS@CeVO4 nanocomposite photoanode for a photosensitive detection of Tyrosine** *Zonguldak Bülent Ecevit University, Faculty of Science, Department of Chemistry, 67100 Zonguldak, Turkey*
15:00- 15:15	Session: Sensor Materials İrem SARIKAYA **(O7)** **Electrochemical sensing of gallic acid based on GCE/TiO2/ZnS nanocomposites** *Sakarya University, Faculty of Science, Department of Chemistry, 54050 Sakarya, Turkey*
15:15- 15:30	Coffee break
15:30- 16:00	Session: Hydrogen and Fuel Cell Science CHAIRs: Dr. Laura Holz and Dr. Martina Kocijan ***Keynote talk*** Dr. Andrei Kovalevsky **(I1)** **MXene-containing composite electrodes for green hydrogen production** *Department of Materials and Ceramics Engineering, CICECO – Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal*
16:00- 16:30	Session: Hydrogen and Fuel Cell Science ***Keynote talk*** Dr. Francisco Loureiro **(I20)** **Ammonia for decarbonizing our world?** *Nanoengineering Research Group, Department of Mechanical Engineering, University of Aveiro, Portugal*
16:30- 16:45	Session: New materials and Advanced materials Dr. Penélope Rodríguez-Zamora **(O1)** **Interaction Mechanisms of Gold, Silver, and Copper Nanoparticles protected by Cysteine: optical properties, environmental applications and biocompatibility** *Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, Mexico City 04510, México*

16:45-17:00	Session: Low Dimension Structures Dmytro Rumiantsev **(O4)** **Interaction between cerium and oxygen films on Mo(112): surface structure and electronic properties** *Institute of Physics of the National Academy of Sciences of Ukraine, Nauky av., 46, Kyiv, 03028, Ukraine*
17:00-17:15	Session: Thin films Prof. Dr. Aleksandr Bagmut **(O44)** **Polymorphous crystallization of amorphous films initiated by electron irradiation: classification and structural-morphological characteristics** *National Technical University "Kharkiv Polytechnic Institute", NTU "KhPI" 2, Kyrpychova str., 61002, Kharkiv, Ukraine*
17:15-17:30	Session: Micro / Nano Materials Dr. Igor Bdikin **(O13)** **Local piezoelectric properties of Di-Leucine dipeptides nanotubes** *TEMA: Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal*
17:30-17:45	Session: Micro/ Nano materials Renata Basto **(O25)** **Reshaping the perifollicular niche to combat Androgenetic Alopecia** *Laboratório Associado para a Química Verde (LAQV), REQUIMTE (Rede de Química e Tecnologia), Department of Chemical Sciences, Faculty of Pharmacy, University of Porto, 4050-313 Porto, Portugal*
17:45-18:00	Session: Engineering & Technology Gabriel Marques **(O35)** **Detection of leakages in closed circuits using luminescent nanoparticles as optical probes** *Departamento de Física and I3N, Universidade de Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal*
18:00-18:15	Session: Engineering & Technology Daniela V. Lopes **(O36)** **Iron electrowinning as a sustainable steelmaking technology: case studies** *CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal*
18:15-18:30	Session: Ceramics Parisa Amirkhizi **(O37)** **Waste Heat Harvesting Using Calcium Cobaltite and Calcium Manganite-Based Thermoelectric Modules** *Department of Materials and Ceramic Engineering, CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193, Aveiro, Portugal*
18:30-18:45	Session: Ceramics Diogo Lopes **(O38)** **Laser Floating Zone processing of SrTiO3 and TiO2 -based thermoelectrics** *CICECO - Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal*
18:45-19:00	***Conference Closing Ceremony***

Poster session, November 22, 2023 (Wednesday), 18:45-19:15

P1	**Mechanical Characterization and Potential Device Fabrication of p-Toluenesulfonate Based Compounds for Nonlinear Optical Applications** Suminda, Sonia *All India Jat Heroes Memorial College, Rohtak, Haryana, India; Baba Mastnath University, Rohtak, Haryana, India*
P2	**Electrochemical behavior of dopamine on the surface of electrodes modified with manganese ferrite nanoparticles** Lizz Gabi Luza Mamani, Edilson Valmir Benvenutti, Tania Maria Haas Costa, Eliana Weber de Manezes, Sabrina Nicolodi, Leliz Ticona Arenas *Laboratory of Solids and Surfaces (LSS), Instituto de Química, UFRGS, CP 15003, CEP 91501-970 Porto Alegre, RS, Brazil; Laboratório de Magnetismo (LAM), Instituto de Física, UFRGS, CP 15051, CEP 91501-970 Porto Alegre, RS, Brazil*
P3	**Oxidation of 1-hexene using supported nano-catalysts under solvent-free conditions** Raiedhah Alsaiari *Empty Quarter research Unit, Department of Chemistry, College of science and art in Sharurah, Najran University, Saudi Arabia*
P4	**Carbon dots as a reinforcement agent in recycled HDPE** Raul Simões, Gil Gonçalves, Teresa Monteiro and Victor Neto *Department of Mechanical Engineering; Centre for Mechanical Technology and Automation; University of Aveiro, Portugal; i3N, Department of Physics, University of Aveiro, Portugal*
P5	**Effect of Cobalt doping on structural optical and electrical properties of sputtered nickel oxide thin films** S. Elmassi, M. Beraich, L. Amiri, M. Bousseta, S. Drissi, A. Abali, L. Nkhaili, A. Narjis, A. Outzourhit *Laboratory of Materials, Energy and the Environment (LaMEE), Faculty of Science Semlalia. Cadi Ayyad University, P. O. Box 2390, Marrakech 40000, Morocco; National school of applied sciences, Ibn Zohr university, Avenue Tamesoult, Agadir 80000, Morocco*
P6	**Structural, Optical and Electrical Properties of Ternary Composites OF BiFeO3-Graphene- KNbO3** S. Vidhya, J. Kishor kumar, A. Durairajan, G. Ramesh Kumar *PG and Research Department of Physics, Arignar Anna Government Arts College, Cheyyar- 604 407, India; I3N-Aveiro-Department of Physics, University of Aveiro, 3810-193, Aveiro, Portugal; Department of Science and Humanities, University College of Engineering Arni-Thatchur-(Anna University, Chennai), 632 326, India*

Plenary lectures

Perspectives of strontium ferromolybdate-based magnetic tunnel junctions

Gunnar Suchaneck*, Gerald Gerlach

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Thin-film strontium ferromolybdate (Sr_2FeMoO_6 – SFMO) is a promising material for applications in room-temperature magnetic tunnel junction (MTJ) devices. MTJs are a promising CMOS-compatible approach to artificial intelligence as they are mimicking key features of biological synapses and neurons with a single device instead of using multiple electronic components. In this work, we consider the main tasks to be solved when creating such devices based on SFMO: (i) selection of an appropriate tunnel barrier material, (ii) role of the interface roughness and its quantification, (iii) influence of the interface dead layer, (iv) appropriate models of the tunnel magnetoresistance (TMR), and (v) promotion of the low-field magnetoresistance in (111)-oriented thin films. We demonstrate that (i) barrier materials with a lower effective electronegativity than SFMO are beneficial since the attraction of more electrons to the SFMO side of the interface increases the occupation of the spin-down states by electrons near the interface thereby increasing the density of states at the Fermi level and, thus, the tunnel current, (ii) diminution of the magnetic offset field (caused by magnetic coupling) requires a wavy surface rather than solely a surface with small roughness, (iii) the interface dead-layer thickness is of the order of 10 nm, (iv) the tunnel magnetoresistance deteriorates due to spin-independent tunneling and magnetically disordered interface layers, and (v) antiphase boundaries along the growth direction promote the negative low-field magnetoresistance. The practical implementation of SFMO-MTJs requires attention to a number of specific aspects: (i) MgO, La_2O_3, $BaTiO_3$, $SrTiO_3$, $LaAlO_3$ and ZnO, are suitable barrier materials, (ii) the interface waviness should be estimated by atomic force microscopy of the constituent layers, (iii) the thickness of the SFMO layer should be much larger than that of the magnetic dead layer at the surface/interface, (iv) the TMR in SFMO-based MTJs may be enhanced by means of (111)-oriented SFMO thin films. The latter is attributed to the influence of antiphase boundaries on charge carrier scattering in SFMO.

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Magnetoactive (multi)functional materials by additive manufacturing

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Multifunctional composites are essential for a large variety of applications, including printed electronics and responsive structures and devices, such as magneto- or piezoresponsiveistive devices, among others. Usually obtained by a combination of functional fillers and an appropriate polymer, these materials allow the development of smart devices for the Industry 4.0 and the "Internet of Things" concepts. These polymer composites are increasingly being implemented by additive manufacturing processing technologies in a variety of shapes, taking advantage of the synergistic combination of their inorganic and organic constituents, and giving rise to a variety of multifunctional responses. The polymer matrix offers advantages in terms of processability, while the filler usually allows to enhance one or more physico-chemical properties.

Due to the variety of effects able to be achieved in structures obtained by additive manufacturing, including permanent magnets, magneto-rheologic, magneto-caloric or magneto-electric materials, among others, magnetoactive functional materials is an area of increasing interest, allowing also improved sustainability and simple integration into devices. Despite its interest, this strategy is particularly challenging based on the requirements imposed to both inorganic functional fillers and functional or passive polymer matrix for a suitable final printable material.

Relevant results, strategies and challenges in the development of specific magnetically active multifunctional materials will be shown, together with applications in the areas of sensors, actuators, biomedicine and energy generation.

Acknowledgements

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Electrodeposition of polyphenols and of nitrogen containing polyphenols

Kevin Ziegler[1,2], Ovidiu Ersen[3], Clément Sanchez[4], Christopher Synatschke[1], Tanja Weil[1] and **Vincent Ball[2]**

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Polyphenols tend to adsorb on all kind of materials and undergo also oxidation followed by precipitation in the solution put in contact with the substrate to be coated. However, The electrodeposition of such molecules can lead to graphene oxide like coatings on amorphous carbon working electrodes without oxidation (and hence loss of active molecules) in solution [1]. Herein the concept of electrodeposition is extended to nitrogen containing phenols, namelly to the isomers of dihydroxypyridine. A strong influence of the nature of the used isomer is found) with the obtention of partially cristalline coatings after the electrodeposition from solutions containing 2,3 and 2,5-dihydroxypyridines. All the obtained coatings are hydrophilic and display marked antioxidant properties. X-ray photoelectron spectroscopy data are used to discuss the structure of the obtained films.

[1] N. Ortiz-Peña, D. Ihiawakrim, V. Ball, S. Stanescu, M. Rastei, C. Sanchez, D. Portehault, O. Ersen, *J. Phys. Chem. Lett*. **2020**, *11*, 9117.

Nanoparticle based piezoelectric energy harvesters

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Piezoelectricity is a unique phenomenon in which by application of force on a piezoelectric material one can generate electric energy. Piezoelectric nanoparticles play pivotal role in developing sustainable green energy alternatives. In the case of nanoparticles, the efficiency of piezoelectric response of a materials can be tailored by controlling the size and morphology of the nanoparticles. Further, the piezoelectric charge coefficient can be enhanced manifold by selective doping e.g. the d_{33} value of pure ZnO, which is less than 10 pC/N, can be increased to a value more than 100 pC/N by various doping and GO incorporation [1-4]. We have synthesized many ZnO based system with different doping and also by hybridization with GO. These piezoelectric systems are used to fabricate flexible nanogenerators. It is demonstrated that electric energy can be generated by various body movements like finger tapping, knee/wrist bending etc. In the present talk the recent results in respect of the fabrication of piezoelectric nanogenerators based on some other piezoelectric nanoparticles, like ZnS, alkali based perovskites, etc will also be described [5].

References

1. Y-doped ZnO nanosheets: Gigantic piezoelectric response for an ultrasensitive flexible piezoelectric nanogenerator, Ceramics International 44 (2018) 8582–8590
2. Tb-doped ZnO:PDMS based flexible nanogenerator with enhanced piezoelectric output performance by optimizing nanofiller concentration, Ceramics International 46 (2020) 24120–24128
3. A review on piezo-/ferro-electric properties of morphologically diverse ZnO nanostructures, Journal of Alloys and Compounds 816 (2020) 152491
4. Remarkably enhanced piezoelectric and ferroelectric characteristics of Er:ZnO upon graphene addition for wearable self-powered piezoelectric sensors MRB 161 (2023) 112149
5. Effect of Nd-doping on 0.95 $(K_{0.6}Na_{0.4})NbO_3$-0.05$(Bi_{0.5}Na_{0.5})$ ZrO_3 ceramics: Enhanced electrical properties and piezoelectric energy harvesting capability JPCS 170 (2022) 110953

Energy, demand for computing power and the Green World:

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Intensive fossil energy consumption, combined with territorial dynamics that tend to concentrate the population in urban areas, poses strong energy challenges to the development of future cities.

The main advantage of energy carriers such as fossil oil, gas, and coal is their high energy density (12,000 Wh/kg in the case of gasoline vs. the current energy density of a car battery of about 250–300 Wh/kg). However, the resulting drawbacks are colossal, and the rate at which renewable energy has grown has been outpaced by ever-growing energy demand. Enormous CO2 emissions mainly originate from the mobility sector and industries.

Recently, the rapidly growing demand for computing power has also started to create a serious energy problem. Until 2012, computing power demand doubled every 24 months; recently this has shortened to approx. every 2 months. Computing power explains 49%-94% of the performance improvements in such domains as weather prediction, protein folding, and oil exploration. But an exponential increase in computing power is needed to get linear improvements in these outcomes. The increasing demand for computing power vastly outpaces improvements made through Moore's law scaling. The exponential increase since 2011 in the costs of training AI models is clearly unsustainable. Machine learning is on track to consume all the energy being supplied, a model that is costly, inefficient, and unsustainable. The cost of powering / cooling a server is now comparable to the purchase cost of the server hardware. Data centres consumed about 8 - 10 % of US electricity in 2019.

To eliminate the use of fossil energy carriers, new alternatives are needed that satisfy some requirements:

- high energy density,
- no CO2 emissions, and
- greater energy efficiencies

as the main rules in the new energy models.

In this talk, I'll analyse the efficiency and applicability of different energy technologies and describe the most promising energy harvesting techniques, including my results in the area.

Mimicking cosmic-dust formation: exotic nanoparticles and vacuum technology

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Cosmic dust grains play an essential role in the emergency of chemical complexity in the universe. In particular, it may catalyze new chemical reactions with the circumstellar and interstellar gases and therefore, dust grain surfaces may contribute to the synthesis of the large variety of molecular species found in the interstellar medium. Albeit its importance, much remains unknown on the cosmic dust formation processes, and high and ultra-high-vacuum technologies may provide an excellent workbench for these studies.

Here, we present the STARDUST machine, an innovative experimental station devoted to the engineering, production, manipulation, processing and *in-situ* analysis of a wide variety of clusters and nanoparticles, particularly designed to mimic the travel of cosmic dust seeds from their formation towards the interstellar medium. Its original design offers unique possibilities for nanoparticle growth with high throughput and controlled size and elemental composition. These highly controlled nanoparticles can also be used in other fields, like catalysis or medicine.

Evaluation of Materials Characteristics Acting as a Carrier For Boron Compounds During Neutron Irradiation and Study of Relevant Boron Compounds (H_3BO_3, B-DTPA) Usually Employed in BNCT-Technique under Neutron Irradiation in a Medically Relevant Reactor Neutron Source

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Experiments on Boron Neutron Capture Therapy (BNCT) carried out at the Institute of Nuclear Techniques (INT), Budapest University of Technology and Economics (TUB), are presented. Relevant investigations are required before designing BNCT for vivo applications. The samples were irradiated using a light water reactor (100 kWt) and Pu(Be) as a portable fast neutron source. The examined materials (carriers) were subjected to neutron beams in the reactor's tangential channel under various experimental settings. The theoretical calculations for the range of expected released particles in various materials, including human tissue, were performed using the Stopping and Range of Ions in Matter (SRIM) software. Samples of relevant boron compounds (H_3BO_3, B-DTPA) usually employed in BNCT were investigated. In this study, a standard ZnS(Ag) detector was used. Graphite blocks were used to modify the neutron beam's characteristics. The portable fast neutron source was placed in a paraffin container to thermalize the fast neutron beam and irradiate the boron compounds. According to experiments and theoretical calculations, the number of protons emitted by tissue-like materials may commit a dose comparable to boron capture reactions. Furthermore, protons have a range that's much greater than alpha particles, which most likely modifies dose distribution in healthy cells surrounding the tumor, which is undesirable in the BNCT technique. The obtained results indicate that the direct measuring method appears to be insufficiently sensitive for detecting the radiation dose committed by the Alpha particles from the ^{10}B (n,α) reaction. As a result, a new approach is required. The measurements and calculations results are in good agreement.

Can nanotechnology tackle state-of-the-art issues?

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ABSTRACT

Smart materials are emerging as an essential component of every aspect that supports the human cycle and the quality human cycle. To meet the demand, the scaling up manufacturing of nanomaterials is a demand that involves the utilization of various toxic chemicals and the further release of unwanted chemicals into the environment. Over time, our ecosystem has continuously been affected adversely that is causing a polluted environment, contaminated human cycle (food, air, and water), and severe diseases. So, as outcomes, we have created several associated problems to solving a problem. If one solution is raising several other problems, then how to manage a balanced system?

In this direction, efforts have been to design and develop green materials that are either bio-derived or and bio-accepted can tackle state-of-the-art issues including environment and health. This is a wide field and can not be covered in a single abstract. To be focused, my research laboratory is exploring nano-enabled approaches to achieve desired sensing and targeted drug delivery – collectively tailored nanotechnology can manage health in a personalized manner [1-7]. To maintain a healthy lifestyle, functional nanomaterials have been tuned to achieve desired photocatalysis for example 1) engineered nano-systems for trapping and eradication of pollutants and microorganisms. 2) anti-bacterial and anti-microbial nano-systems to support green technology. 3) nano-enabled sensing technology to detect a targeted biomarker (for example SARS-CoV-2, Zika, etc.) at a low concentration. These sensing prototypes have been supported by the Internet-of-Things (IoT) and Artificial Intelligence (AI) to perform sensing at point-of-care applications and bioinformatics analysis to understand and manage diseases. 4) explore engineered biocompatible materials to achieve targeted drug delivery wherein delivery and release of a drug should be in a controlled manner. This approach has been suggested as future therapy where s medicine will be performed according to the patient profiling i.e., a personalized nanomedicine approach.

Overall, it is anticipated that nano-enabled approaches are successfully playing a good role in tackling serious issues that are a threat to a healthy lifestyle. But at the same time, efforts must be made to explore this nano-system in a green manner (green chemistry and technology) according to the goals of sustainability. Additionally, a focus is also suggested to make new policies to regulate and monitor all types of nanomaterials investigated for applied applications and only bio-acceptable materials must be promoted.

REFERENCES

1. Chakraborty, U., Kaur, G., Rubahn, H.G., Kaushik, A., Chaudhary, G.R. and Mishra, Y.K., 2023. Advanced metal oxides nanostructures to recognize and eradicate water pollutants. Progress in Materials Science, 139, p.101169.
2. Kaushik, A.K. and Dhau, J.S., 2022. Photoelectrochemical oxidation assisted air purifiers; perspective as potential tools to control indoor SARS-CoV-2 Exposure. Applied Surface Science Advances, 9, p.100236.
3. Tyagi, N., Sharma, G., Kumar, D., Neelratan, P.P., Sharma, D., Khanuja, M., Singh, M.K., Singh, V., Kaushik, A. and Sharma, S.K., 2023. 2D-MXenes to tackle wastewater: From purification to SERS-based sensing. Coordination Chemistry Reviews, 496, p.215394.
4. Ataei Kachouei, M., Kaushik, A. and Ali, M.A., 2023. Internet of Things-Enabled Food and Plant Sensors to Empower Sustainability. Advanced Intelligent Systems, p.2300321.

5. Kaushik, A.K., Dhau, J.S., Gohel, H., Mishra, Y.K., Kateb, B., Kim, N.Y. and Goswami, D.Y., 2020. Electrochemical SARS-CoV-2 sensing at point-of-care and artificial intelligence for intelligent COVID-19 management. ACS Applied Bio Materials, 3(11), pp.7306-7325.
6. Kaushik, A., Jayant, R.D., Bhardwaj, V. and Nair, M., 2018. Personalized nanomedicine for CNS diseases. Drug Discovery Today, 23(5), pp.1007-1015.
7. Varahachalam, S.P., Lahooti, B., Chamaneh, M., Bagchi, S., Chhibber, T., Morris, K., Bolanos, J.F., Kim, N.Y. and Kaushik, A., 2021. Nanomedicine for the SARS-CoV-2: state-of-the-art and future prospects. International journal of nanomedicine, pp.539-560.

Formation of multipolar states in layered $CuInP_2S_6$ ferrielectrics

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$CuInP_2S_6$ (CIPS) is a van der Waals layered crystal in which the ferrielectric ordering is preserved as the thickness is reduced to a few layers [1], making it a viable option for advanced nanoelectronic applications. Through a DFT-based molecular dynamics simulation of Cu cation flipping dynamics and In cation displacive dynamics within the CIPS crystal lattice, a dipole ordering dependent on temperature is confirmed. The simulation indicates the presence of a double-well local potential for Cu cations and a three-well local potential for In cations. These shapes of the local potentials are induced by the second order Jahn-Teller effect [2]. In addition, a quantum anharmonic oscillators (QAO) model was used to describe the temperature evolution of the spatial distribution of Cu and In cations within the structural layers. At positive pressures, the cooling process results in a first-order transition from a paraelectric phase to a ferrielectric phase, which is determined by the higher energy of the side wells in comparison to the central well of In cation's local potential. The named side wells undergo stabilization with the rise of negative compression, resulting in a second-order transition from paraelectric-to-ferrielectric phase. Inside the ferrielectric phase, a first-order transition between states with different values of spontaneous polarization can be observed. Polarization switching in CIPS at different temperatures and pressures demonstrates the presence of single, double, or triple hysteresis loops. The predicted triple loops under stretching external pressures are correlated with the observed loops under the influence of internal chemical pressure, which appears at the partial substitution of copper by silver [3] or sulfur by selenium [4]. The results of our modeling calculations are in good agreement with the mean-field analysis of the $CuInP_2S_6$ phase diagram and the peculiarities of the polarization switching [5].

References

[1] A. Belianinov, Q. He, A. Dziaugys, P. Maksymovych, E. Eliseev et al., *Nano Lett.,* **15**, 3808 (2015).
[2] Y. Fagot–Revurat, X. Bourdon, F. Bertran, V.B. Cajipe and D. Malterre, *J. Phys.: Cond. Matter.,* **15**, 595 (2003).
[3] I. Zamaraitė, A. Dziaugys, Y. Vysochanskii, J. Banys, *Lithuanian Journal of Physics,* **62**, 229 (2022).
[4] V. Samulionis J. Banys, Yu. Vysochanskii, *Ferroelectrics,* **379**, 69 (2009).
[5] A.N. Morozovska, E. A. Eliseev, Yu. M. Vysochanskii, D.R. Evans, *Phys. Rev. Appl.,* **19**, 054083 (2023).

Functionalized PEI Coated Magnetic Nanoparticle Sorbents for Removal of Lead from Aqueous Solution

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Polyethylenimine-coated magnetic nanoparticles functionalized with difference organic-inorganic moieties were synthesized via a simple hydrolysis route. A new generation of magnetically separable adsorbents decorated with new functional groups was synthesized to reach high stability and adsorption capacity and were employed in the removal of Pb(II) from aqueous solutions.

MNPs were first coated with PEI by covalently grafting PEI on the surfaces of Fe_3O_4 followed by functionalization with organic and inorganic moieties having various electron donor sites, i.e. N and O or S. These adsorbents were employed in Pb(II) ion removal from aqueous solution and the concentration of metal ions adsorbed was determined. Coating and functionalization of Fe_3O_4 not only render the adsorbents hydrophilic leading to a reduction of adsorption during wastewater treatment but also equally provide several hydroxyl, thiol and thiocarbamate groups, which may act in synergy to coordinate or chelate the Pb(II) metal ions. Consequently, this increases their absorption capacity more rapidly and may easily be removed from the solution. The nanoadsorbents can be reused without affecting their removal capacity.

A very effective uptake of Pb(II) (98.1% of 25 mg L^{-1} Pb(II)) was achieved with an adsorbent dose of 10 mg, a contact time of 60 min and at a pH of 6.5. Equilibrium data for isothermal, kinetic and thermodynamic studies indicate that the process of adsorption fitted well with the Langmuir adsorption isotherm model. The kinetics of adsorption proceeded through a pseudo-second-order rate while the thermodynamic parameters indicated that the process was spontaneous and endothermic.

The proposed mechanism of formation of the materials is presented and discussed. Furthermore, the effects of different parameters including the concentration of Pb(II) ions, contact time, pH and the amount of adsorbent on the capacity of adsorption of Pb(II) ions by the prepared nanocomposites were explored. The reusability as well as adsorption mechanism of Pb(II) ions were also evaluated

Invited speakers

I1. MXene-containing composite electrodes for green hydrogen production

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Growing energy needs require sustainable methods for energy conversion and storage. The intermittent nature of renewable energy sources challenges their full integration into electric grids. One promising solution is utilizing this energy for water electrolysis, producing green hydrogen, a zero-carbon, high-energy fuel with water as the only by-product of energy release.

The emergence of new multifunctional materials continuously increases the expectations for the technologies advancing the hydrogen economy, like alkaline electrolysis. MXenes, a family of two-dimensional (2D) transition metal carbides, nitrides and carbonitrides based on abundant constituents, has been discovered as an exciting candidate for these applications [1]. The water adsorption on MXenes is exothermic and facilitates its dissociation [2]. This fact makes them very promising as electrocatalysts for electrochemical water splitting and, in particular, for hydrogen evolution reaction (HER) in an alkaline medium, where water dissociation is a rate-limiting step [3].

Several critical issues limit the broad applications of MXenes, including the use of HF for their preparation and their low ambient stability, mainly related to the oxidation in the presence of water and oxygen and microstructural degradation. This presentation will highlight recent advancements in developing reliable and inexpensive electrodes for hydrogen production, promoted by a facile method of MXene synthesis and incorporation. Various composite electrode concepts will be reviewed and discussed.

References

[1] M. Naguib, M. Kurtoglu, V. Presser, J. Lu, J. Niu, M. Heon, L. Hultman, Y. Gogotsi, M.W. Barsoum, *Advanced Materials*, **vol. 23**, 4248-4253 (2011).
[2] J. D. Gouveia, Á. Morales-García, F. Viñes, F. Illas, J. R. B. Gomes, *Applied Catalysis B: Environmental*, **vol. 260**, 118191 (2020).
[3] N. Mahmood, Y. Yao, J. W. Zhang, L. Pan, X. Zhang, J. J. Zou, **vol. 5**, 1700464 (2018).

I2. Improving the thermal management of electronic devices with diamond films

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The thermal management of electronic components has become a requirement transverse to several applications. Operation at high temperatures impairs the components reliability and may be accompanied by an increase of the electrical resistance, resulting in higher losses and lower efficiency. Different techniques can be used to promote the transfer of heat from the active regions in a device to the package, where it can be ultimately dissipated to the heat sink or external environment. One of the possibilities is the use of materials with high thermal conductivity within the package itself, as a substrate material or as a chip-carrier. Due to its high breakdown electric field and thermal conductivity, diamond can be considered the ultimate thermal management material; it is available in the form of plates and can be deposited on non-diamond substrates, which allows for different possibilities integration architectures – as substrate, as chip-carrier and even as board. This talk will review some successful examples of integration of diamond and electronic devices such as disk lasers and high electron mobility transistors (HEMTs).

I3. Photochemistry of Triplet-State and Exploitation in Solid-state Photo-switching

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The triplet state in photochemistry is Pauli's spin-forbidden state triplet due to quantum restrictions of accommodating two electrons having the same spin in the same orbital. However, stable excited triplet-states are possible in organic molecules even at room temperature with suitable molecular design to surpass the spin restrictions. For example, heavy metal-porphyrins and complexes. While it can be exploited for many photonic applications (photovoltaics, photo-pharmacology, optogenetics, etc.), the efficiency is challenged by molecular oxygen that we breathe which also exists in triplet form in its ground state. [1] In this talk, I will talk about our recent research on triplet-sensitized photoisomerization (TSP).[2] However, the realization of efficient TSP materials in the solid-state for practical application faces issues of chromophores aggregation and deactivation of excited triplets by dissolved oxygen molecules and conformational constraints. We overcame these issues by developing a generalized approach of biopolymer surfactant-chromophore co-assembly where TSP chromophores are confined inside surfactant nano-domains coated with thick fiber networks of biopolymers in hydrogels or bioplastic frameworks (Fig. 1). Employing this approach, we have realized a series TSP material that can convert azobenzene upon excitation in the broad excitation range from 640 to 740 nm.

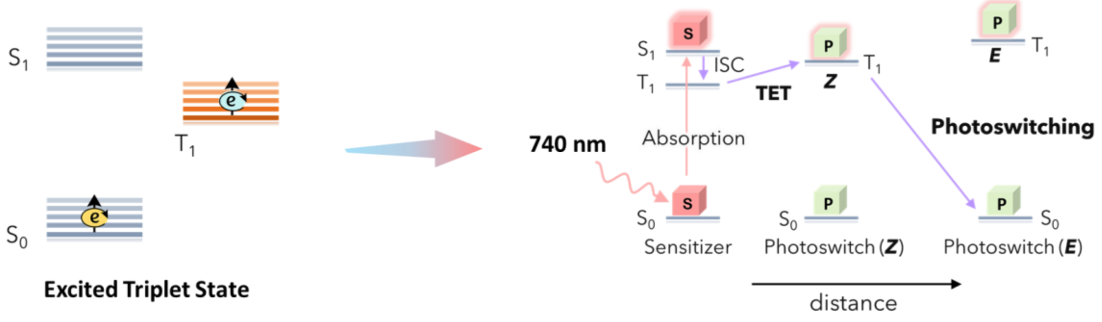

Fig. 1. Air Stable triplet-sensitized photoisomerization in confined nano-domains

References

[1] **P. Bharmoria**,* H. Bildirir and K. Moth-Poulsen,* Triplet–triplet annihilation based near infrared to visible molecular photon upconversion, Chem. Soc. Rev. **49**, 6529–6554 (2020).

[2] **Pankaj Bharmoria**,* Shima Ghasemi, Fredrik Edhborg, Raúl Losantos, Zhihang Wang, Anders Mårtensson, Masa-aki Morikawa, Nobuo Kimizuka, Ümit İşci, Fabienne Dumoulin, Bo Albinsson, Kasper Moth-Poulsen,* Far-Red Triplet Sensitized Z- to - E Photoswitching of Azobenzene in Bioplastics. *Chem. Sci.*, *13*, 11904-11911 (2022).

I4. Piezoelectric nanogenrators for self-powered Internet-of-Things (IoT) devices

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Due to the recent miniaturization of electronic devices, implementation of the internet of things (IoT) is accelerating at very high rate. Wireless sensing technology is ideal for many industrial applications such as condition monitoring and smart appliance applications. In the era of IoT, hundreds or even thousands of sensors and portable electronics are deployed in a remote area. Continuous replacement of the batteries for these huge number of electronic devices is time consuming and inefficient. Therefore, energy harvesting technology such as piezoelectric nano generators (PENGs) is attractive alternative to traditional rechargeable batteries for providing electric power to low-energy portable devices. The aim of this paper is to present current status and future challenges related to PENGs to supply sufficient power to IoT devices.

I5. Impedance modulated dielectric and magneto dielectric properties of Lead free KNN and $NiTiO_3$ based composite ceramics

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A composite ceramic based on $(K_{0.5}Na_{0.5}NbO_3)$-$(NiTiO_3)$ was prepared using ferroelectric $(K_{0.5}Na_{0.5}NbO_3)$ and a transition metal Ti-based perovskite system by the solid-state reaction method with different mol% of x, representing the concentration of $NiTiO_3$ (where x = 0.025, 0.050, 0.075, 0.10). Preliminary structural studies were carried out by X-ray diffraction and Raman Spectroscopy at room temperature. The composite showed orthorhombic symmetry from the XRD and Raman at room temperature. The SEM images of the composites revealed the presence of both cuboidal-shaped and large agglomerated grains. All of the temperature data and the frequency dependence of the impedance were utilized to characterize the sample's electrical conduction, revealing NTCR (Negative Temperature Coefficient Resistance), typically encountered in the case of semiconductors and exhibiting a significant divergence from the ideal Debye-type behavior. The magneto-dielectric property initially increased with x and was found to be a maximum of ~40% for x = 0.10. Lead-free KNN-based and transition metal-based composites may provide an opportunity for the miniaturization of environmentally friendly magneto-dielectric (MD) devices.

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I6. Water Pollution Control and Hydrogen production using Multifunctional Organic & Inorganic Photocatalyst

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Complex organic dyes and pigments are serious waste which damages the ecosystem as well as aquatic life. Researchers are working to overcome this serious issue for many years, but to developed cost-effective and eco-friendly method is unsolved challenge. Of late, inorganic based photocatalysis helps to treat industrial wastewater to some extent. Various inorganic semiconductor photocatalysts with high efficiency have been reported with different dyes degradation study.

We have synthesized 6,13-Pentacenequinone (PQ) an intermediate required to synthesize Pentacene which is well known organic semiconductor. After complete characterization we explored PQ for Industrial Dye degradation and photocatalytical H_2S splitting for the first time. We also synthesized the composite system of PQ-TiO_2 with inorganic semiconductor photocatalyst. Recently a report of PQ-MoS_2 photocatalyst also covers the water splitting area. This organic PQ photocatalyst has high potential in photocatalysis field which can be utilized for the clean environment and for Hydrogen generation.

I7. Effect of swift heavy ion irradiation on lithium borate glasses

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Lithium borate (LBO) glasses of the composition $10LiO_2$-$90B_2O_3$were prepared by melt quenching technique. The pristine LBO glasses were irradiated using 100 MeV Ni^{7+} ion of 1 pnA beam current for different fluences such as 1×10^{11}, 5×10^{11}, 1×10^{12}, 5×10^{12} and 1×10^{13} ions/cm^2. The LBO glasses were characterized before and after ion irradiation to analyse the changes induced by ion irradiation on the density, structural, optical, refractive index and morphological properties. The SRIM 2008 was used to calculate the electronic and nuclear energy losses in LBO glasses due to 100 MeV of Ni^{7+} ion irradiation. Optical basicity, ionicity, the molar volume of oxygen, oxygen packing density, boron-boron separation and bond density were calculated. XRD and FE-SEM confirm the transformation of LBO glasses from amorphous to polycrystalline nature that arises from deformation that causes nucleation[1]. Rietveld refinement shows that the irradiated LBO glasses possess a monoclinic structure of lithium pentaborate pentahydrate($B_5H_{10}LiO_{13}$). The surface morphological changes by the formation of cubic crystallites were witnessed using FE-SEM. Raman spectra were recorded for the pristine and unirradiated samples and transitions are discussed. The direct band gap of pristine and ion-irradiated LBO glasses decreases from 2.73 to 2.55 eV. The Urbach energy was found to decrease from 0.59 to 0.42 eV after ion irradiation[2]. After irradiation, the FTIR spectra show the creation of non-bridging oxygens (NBO) by the formation of BO_4 units at the expense of BO_3 units[3].

References:

1. *C. L. Dube, M. C. Stennett, S. Akhmadaliev and N. C. Hyatt, Journal of Non-Crystalline Solids: X (2020) 100055.*
2. *E. M. Haily, L. Bih, M. Jerroudi and A. El Bouari, Materials Today: Proceedings (2021) 10.*
3. *J. Li, Y. Sun, Z. Li and Z. Zhang, ISIJ International (2016) 752.*

I8. A new approach to key challenges in additive manufacturing by laser sintering

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Additive Manufacturing (AM) is a powerful collection of techniques which has the potential to become a reliable method for the manufacture of complex and accurate parts. However, some key challenges still limit their widespread application. The key challenges addressed here, specifically for the Laser Sintering AM process are: (1) limited availability of different materials, (2) inconsistent or poor properties and (3) surface quality, each of which is currently still restricting the functions of the end-use parts.

In some cases, nanoclay reinforcement of polymers has been shown to provide performance benefits, improving part quality and offering new applications. However, the dispersion of those nano-sized materials still remains a critical issue for the preparation of Laser Sintering nanocomposites. Plasma treatment is used to reduce agglomeration and improve nanoclay dispersion (addressing point no. 1). No significant deterioration in LS processibility was observed and complex LS parts could be produced when including the nanoclay. SEM images of the cross-sections of the fabricated parts that the layer by layer structure were successfully consolidated and relatively uniform. In addition, the introduction of the plasma treated nanoclay was found to improve the elastic modulus of the LS composite parts (addressing point no. 2). Most notably however, a substantially improved surface quality in part’s appearance and microstructure was found as a result of incorporating plasma treated nanoclay compared to the nontreated nanoclay (addressing point no. 3).

I9. Nanotechnological Methods to Characterize the Allende Meteorite

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Nanotechnological methods are critical in recognizing nanotubes, graphene, fullerenes, and nanorods in meteoritic materials. By studying these nanomaterials in meteorites, scientists might gain valuable insights into the origins of our solar system, as well as the potential use of these materials in new technologies. Nanotechnological methods, such as scanning electron microscopy (SEM) and Atomic Force Microscopy (AFM), allow scientists to image and analyze these nanomaterials at the molecular and atomic levels. For example, nanotubes are cylindrical structures composed of carbon atoms considered to be relevant for their chirality, while fullerenes are spherical molecules of carbon atoms, and nanorods might be composed of NiFe solids with magnetic properties. Understanding the presence and distribution of nanomaterials in meteoritic materials is of great importance to our understanding of the formation and evolution of our solar system and ancient Earth. These nanomaterials such as those found in the Allende meteorite likely formed under extreme conditions, such as in the stellar environment or during the early stages of our solar system's formation. Furthermore, the possible unique properties and composition of such nanomaterials make them highly desirable for use in new technologies.

In conclusion, nanotechnological methods play a vital role in recognizing nanotubes, fullerenes, and nanorods in meteoritic materials, and in this specific case, magnetic nanomaterials in the Allende meteorite. This knowledge is crucial for understanding the formation and evolution of our solar system, as well as for increasing the potential of the development of new technologies and catalytic possible ways of these complex nanostructures. Further advancements in our understanding of meteoritic nanoscale materials and their applications in various industries are of main relevance.

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I10. Graphene-based nanocomposites for environmental and health applications

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Carbon, a fundamental element, has a fascinating history dating back to prehistoric times when humans first encountered it in the form of charcoal. Notably, one of our earliest uses of carbon was for artistic expression in ancient cave paintings.[1] The emergence of nanotechnology has revolutionized our understanding of carbon materials. Remarkable advancements in synthesizing carbon nanomaterials have opened up exciting possibilities capable of addressing various societal challenges.

Graphene-based materials (GBMs) have emerged as a particularly promising area of study. Their exceptional properties, including a high surface area, outstanding biocompatibility, and the capacity to be tailored with various structures, render them well-suited for a diverse array of applications.[2] These applications span from targeted drug delivery and bioimaging to the cutting-edge realm of photothermal therapy.[3] Furthermore, GBMs have demonstrated their potential in water purification and remediation. Their outstanding adsorption capabilities, particularly in removing pollutants like heavy metals and organic compounds, offer viable solutions to urgent water quality challenges.[4] In the upcoming discussion, I will delve into our ongoing research efforts focused on developing novel nanostructured GBMs, with a specific emphasis on their applications in cancer nanomedicine and water remediation. Additionally, I will share my vision for the future of this dynamic and rapidly evolving field of GBMs.

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[1]R. Moliner, Carbon, (2016) 2-5.
[2]G. Gonçalves, Graphene-based Materials in Health and Environment, 2019, Springer Cham, ISBN 978-3-319-45639-3
[3] C. I. M. Santos et al., ACS Appl Nano Mater, 2021, 4, 13079–13089.
[4] A. Bessa et al, Chem Eng J, 2020, 398, 125587.

I11. Enhancing Light Efficiency for Horticulture with Rare-Earth and Transition Metal-Doped Phosphors

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In the realm of contemporary horticulture and plant growth control, the efficient utilization of light plays a pivotal role. This presentation focuses on the synthesis and characterization of phosphor materials doped with rare-earth (RE) / transition metal (TM) ions, with the objective of enhancing their light-emitting properties. The research encompasses the creation and thorough analysis of both singly doped and co-doped phosphor samples, employing a range of characterization techniques.

Our investigation reveals that these doped phosphor materials exhibit robust photoluminescence, which is a critical factor for their potential applications in horticulture lighting. Importantly, in the case of the co-doped samples, it is observed that the emissions of RE and TM ions occur independently, without any mutual quenching or energy transfer mechanisms. This independence is significant as it allows for precise control of the emitted light, a valuable feature for tailored lighting solutions in horticulture.

Overall, the results of our study underscore the considerable potential of the doped phosphor materials for various applications. One of the most promising applications is in solid-state lighting, which can be tailored to provide the specific light spectra required for optimized plant growth. The ability to control and fine-tune the emitted light makes these materials a valuable asset in the pursuit of efficient and sustainable horticulture practices.

References

[1] S.K. Jakka, M.M.P. Silva, M.J. Soares, K. Pavani, RSC Advances, **13,** 31314A (2023).

I12. Structural and photoluminescence studies rare earth doped metasilicate phosphor for solid state lighting applications

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Solid-state lighting (SSL) technology has attracted extensive attention due to its wide applications in various fields such as display devices, and bio-imaging. This technology has fundamentally altered the production and utilization of lighting in all facets of our lives which enables a huge reduction in domestic and global energy consumption. Rare earth ions doped phosphors were extensively studied due to the strategy that involves a binary combination of blue LED and yellow phosphor to produce white light lacking in the red component. Therefore, an investigation of structural and luminescent properties to develop red phosphors is very much attractive.

In this talk, the importance of the synthesis of red phosphor and the description of energy transfer-induced color tunability behaviour of rare earth bi-activated metasilicate phosphor for luminescent device applications will be discussed. It is commonly known that commercial w-LEDs are fabricated by coating a yellow emitting YAG: Ce^{3+} (Ce^{3+} doped yttrium aluminium garnet) phosphor with a reasonably broad spectrum on blue emitting InGaN LED chip. One such fabricated w-LED shows a deprived value of color rendering index and correlated colour temperature caused by the dearth of red colour emitting component. In order to achieve sufficient CRI and lower CCT with improved luminous stability, researchers and scientists have to delve into an alternative approach with the suitable amalgamation of RGB (red: R, green: G and blue: B) mono phase phosphor. Solid state reaction methodology has been adopted to synthesize bi-activated thermally persistent metasilicate phosphors and investigate their structural, morphological and luminescent characteristics. The illumination shift has been observed from yellow to red region with varying the activator ions concentration and also colour tunability by altering the excitation energy. Further, temperature dependent studies have been carried out to analyse the thermal stability of the phosphor. In conclusion, the potential utility of rare earth bi-activated metasilicate phosphors with tremendous thermally stable behavior with flexible color tunability for w-LED applications will be demonstrated.

I13. Nanofluids for heat transfer enhancement: challenges and opportunities

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- Abstract

Efficient heat transfer is the key to achieve sustainable and economic thermal systems, such as solar collectors, heat exchangers, automotive radiators, electronic devices, just to name a few. Moreover, nanofluids are enticing choices to couple with such heat transfer applications due to their excellent thermophysical properties, rendering miniaturization of some of these systems feasible. Nevertheless, nanofluids' long-term stability is paramount to guarantee the fluid exceptional thermal properties. A vast amount of research on nanofluids has been carried out during the past 15 years, but from a revision on the most recent literature on the field, it can be depicted that a systematic study, comprehension and, perhaps, attention on the nanofluids stability fails to be reported. The nanofluid stability mechanism, stability characterization technology, factors affecting stability and stability enhancement method simply do not prevail in the great majority of the studies involving the production and characterization of nanofluids. The latter, greatly contributes to the lack of reproducibility of the reported data, considerably increasing this technology time-to-market. It seems, therefore, fundamental, to summarize current advances in the study of nanofluids, but also to review stability mechanisms, its assessment and enhancement procedures, as well as how it affects the nanofluid thermophysical properties.

- Introduction

With the increasing requirements for heat transfer enhancements in the industrial fields, a new concept of nanofluid was proposed in 1995 [1]. The nanofluid is a stable suspension obtained by mixing nanoparticles in a base fluid, such as water, ethylene glycol, and oil. Compared with traditional fluids, the random movement of nanoparticles in a nanofluid enhances the turbulence intensity of the fluid, reduces thermal resistance, and dictates excellent thermal performance. The researchers have been attracted to investigations on the heat transfer performance of nanofluids on several applications. [2].

- Stability

. The preparation of stable nanofluids is fundamental for improving the thermal performance of these systems [3]. The ideal nanofluids detain high thermal conductivity, low viscosity, good stability, and should be affordable [4]. However, the stability of nanofluids depends upon the nanoparticles and the base fluids used. Nanoparticle aggregation is used as the common criterion for evaluating the stability of nanofluids, which depends on the thermodynamic characteristics and the total interaction between the particles [5]. Nanoparticles (<1nm) collide due to the Brownian motion, forming secondary particles under the impetus of attraction. The collision of secondary particles induces aggregation essentially due the nanoparticles high surface area. After reaching a certain volume, aggregation causes sedimentation and, hence, suspension instability

[6]. In order to avoid the poor stability of nanofluids, it is necessary to suppress the high surface effect and chemical activity of nanoparticles. For the small size, the stability of nanoparticles in suspension is mainly affected by the van der Waals forces [7], electrostatic forces [9], gravitational forces [8]. The first two playing a greater role. The van der Waals force is inversely proportional to nanoparticle diameter, therefore nanoparticles have a robust van der Waals force due to their small size. According to the theory proposed by Derjaguin, Landau, Vewey, and Overbeek (DLVO), it is a dynamic balance between the van der Waals force and the electrostatic force [10]. When the electrostatic force generated by the electric double layer around the particles is greater than the van der Waals force between the particles, the nanoparticles are uniformly dispersed in the medium to obtain the nanofluid with good stability [11].

- Preparation Methods

. According to the mechanism of dispersing nanoparticles, nanofluids are prepared using two methods, i.e., the one-step method [12] and the two-step method [13]. The stability of nanofluids is affected by material type, the temperature of nanofluids, size, shape, and concentration of nanoparticles [12,13]. Usually, high particle density and large particle size cause poor dispersion on nanofluids. The collision probability of nanoparticles is positively correlated with the volume fraction of nanofluids, which leads to strong aggregation and low stability of nanofluids [17]. The stability of nanofluids is improved using chemical and physical methods. In physical methods, the particle size of nanoparticles is reduced mainly using ultrasonic oscillation and nanofluids agitation. In chemical methods, the pH value of the liquid is adjusted, and various surfactants are added to modify the surface of nanoparticles [13]. These methods change the surface activity of particles and destroy the mutual attraction among nanoparticles in the aggregation process.

- Challenges and opportunities

The stability of nanofluids is to be comprehensively addressed and reviewed. Moreover, the literature is reviewed to reveal a gap in references related to stability of nanofluids. The preparation method of nanofluid, thermophysical properties affecting stability, stability mechanism, stability characterization technology, and stability enhancement method are summarized to indicate that the stability of nanofluids is related to the method of nanofluid preparation, particle concentration, surfactant used, ultrasonic oscillation, pH, and surface modification. In addition, the direction and strength of the magnetic field may affect the stability of particular nanofluids, namely ferromagnetic fluids. The stability of hybrid nanofluids is affected by the synergistic interaction between different nanoparticles. The literature has revealed considerable effort put on the preparation, thermophysical properties characterization, and applications of several nanofluids. It is here intended to highlight the enticing potential of these systems to enhance heat transfer, but also to establish the research direction to solve the nanoparticle aggregation, by analyzing the effect of various parameters on the stability of nanofluids. Furthermore, it is intended to present and review theories and methods to address the aggregation of nanofluids offering the possibility to enhance the system efficiency and achieve largescale applications of nanofluids.

References

[1] S.U.S. Choi, J.A. Eastman, Enhancing thermal conductivity of fluids with nanoparticles, Argonne National Lab.(ANL), Argonne, IL (United States), 231; 99-105A, (1995).

[2] K. Pushparaj, W.C. Liu, A. Meyyazhagan, A. Orlacchio, M. Pappusamy, C. Vadivalagan, A.A. Robert, V.A. Arumugam, H. Kamyab, J.J. Klemeš, T. Khademi, M. Mesbah, S. Chelliapan, B. Balasubramanian, Energy, 240 (2022)

[3] M. Sandhya, D. Ramasamy, K. Sudhakar, K. Kadirgama, M. Samykano, W.S.W. Harun, G. Najafi, M. Mofijur, M. Mazlan, Sustain Energy Technol Assessments, 44 (2021)

[4] K. Jafari, M.H. Fatemi, A.P. Toropova, A.A. Toropov, Chemometr Intell Lab Syst, 222 (2022)

[5] Borzuei M, Baniamerian Z.. Int J Heat Mass Tran;150:119299 (2020).

[6] Ueki Y, Oyabu T, Shibahara M.Int Commun Heat Mass Tran 117:10480, (2020).

[7] Alsarraf J, Al-Rashed AAAA, Alnaqi AA, Shahsavar Goldanlou A. Powder Technol, 379:537–46. (2021)

[8] Mehryan SAM, Goudarzi P, Hashem Zadeh SM, Ghodrat M, Younis O, Ghalambaz M. Int Commun Heat Mass Tran,**126**:105345, (2021).

[9] Mahdavi M, Sharifpur M, Meyer JP. Powder Technol, **307**:153–62, (2017).

[10] Verwey EJW, Overbeek JTG. J Colloid Sci, **10**:224–5, (1955).

[11] Qiao A, Cui M, Huang R, Ding G, Qi W, He Z, Klemeˇs JJ, Su R. Carbohydr Polym:**272** (2021).

[12] Ding J, Zhao H, Yu H. Carbon,**171**:29–35, (2021).

[13] Zheng D, Wang J, Pang Y, Chen Z, Sunden B. Therm Sci; **24**:3601–12,(2020).

I14. Growth and structural characterization of h-LuMnO3 thin films deposited by MOCVD

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Rare Earth manganites (*R*MnO3) systems broadly studied as ceramics and single crystals, can present additional degrees of freedom as thin films,due to substrate induced strain and interface modifications, opening practical pathways for engineering multifunctional devices. Thin films deposition by chemical vapor methods [1] like MOCVD have some advantages of lower cost, versatility of precursors composition and control of films stoichiometry, when compared to physical-based techniques, such as pulsed laser deposition [2], RF sputtering, molecular beam epitaxy. In this work, are explored the MOCVD conditions to synthetize the hexagonal LuMnO3 phase onto SiO_2 glass and Si(100)\$SiO_2$\$TiO_2$\Pt(111) substrates. Main parameters investigated are metalorganic precursors ratios, substrate temperature, atmosphere, and annealing effects. Detailed analysis of the films was carried out by XRD, SEM, EDS, PFM, RMS, and Diffuse Reflectance. Results confirmed that formation of the $P6_3cm$ *h*-LuMnO3 single phase [3] can be achieved within $0.93 < |Lu|/|Mn| < 1.33$ precursors molar ratio; crystallization occur at 800 °C; deposition and annealing should be performed in Argon, accounting only the residual O_2 as sufficient to oxidize the film. The films exhibit a relatively narrow band gap <1.5 eV, within the values reported for the *h*-LuMnO3 system [4]. Such low band-gap ferroelectric materials are seen with potential for the development of next-generation photo-ferroic devices.

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References

[1] Y.R.-Barcelay, J.A. Moreira, G.G.-Aguilar, A. Almeida, J.P. Araujo, J.P. Cruz, *J. Electrocer.* **26**, 2011, 44–55.
[2] A.M. Zhang, H.F. Cao, X.X. Pan, J.J. Zhu, X. S. Wu, *Thin Solid Films* **750**, 2022, 139186.
[3] F. Figueiras, D. Karpinsky, P.B. Tavares, S. Das, J. Leitão, E. Bruck, J.A. Moreira, V. Amaral, *Phys.Chem.Chem.Phys.* **18**, 2016, 13519
[4] Y. Sheng, I. Fina, M. Gospodinov, J. Fontcuberta, *Appl. Phys. Lett*. **118**, 2021, 232902.

I15. Composite/hybrid coatings as an innovative way to improve electrodeposited materials

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The innovative ways for coatings protection and repair have a very important role in modern technology and industry. The repair procedures of the coating that can be performed in situ and, at the same time, can take into account demands for energy saving and sustainability have gained increasing interest. In this view, the elaboration of hybrid/composite materials has been extensively investigated. The combination of a wide variety of compositions and production processes allowed the use of these materials in different applications like coatings for corrosion and wear protection. Production processes for such coatings are quite versatile and not limited to micro-arc oxidation, electrodeposition, sol–gel, chemical/physical vapor deposition, electrospark deposition (ESD).

In our study, the hybrid coatings were obtained using a combination of ESD and electrodeposition methods. The ESD technique is a low-heat-input process that has great potential for coating applications and the restoration of damaged high-value parts. The electrodeposition was used in order to reduce the roughness of the ESD coatings, which is a common issue of the ESD process. Hence, the micro-leveling power of several electrolytes for Ni, Fe-W, Fe, and Cr electrodeposition was evaluated. The maximum leveling effect was detected for Ni electro-plated from the Watts electrolyte.

Thus, the novel hybrid coatings based on an ESD layer and a subsequent layer of electrodeposited Ni were obtained and analyzed in comparison to ESD coatings for wear and corrosion behavior. For all the studied cases, the corrosion resistance of the hybrid coatings was higher than for their ESD counterparts and close to electrolytic chromium.

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I16. Paper-based microfluidic fuel cells fed by eco-friendly organics

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Microfluidic fuel cells are emerging miniaturized systems that convert chemical energy from fuel into electric energy by coupling a spontaneous redox reaction [1]. Among the miniaturized energy converters, paper-based microfluidic fuel cells (PµFCs) fed by eco-friendly organics from biomass appear as flexible, self-pumping, lightweight, disposable, and sustainable devices to produce energy. PµFCs have gained attention after important applications, such as that to power pregnancy tests [2]. The major challenge is to deliver useful energy to power the small devices but at a low cost and environmentally friendly. These features justify them being disposable. Therefore, investigating eco-friendly reactants and low-cost catalysts is key to transit towards commercial systems. This talk displays an overview of recent advances from the Electrochemistry Research Group at UFMS-Brazil regarding PµFCs. We reported PµFCs equipped with Pt/C on carbon paper (CP) anode, a metal-free CP cathode fed by the following biomass-derived; methanol, ethanol, ethylene glycol, and glycerol fuels in an alkaline medium [3]. The cathode was fed by sodium persulfate in an acidic medium. These unprecedented biomass-fed PµFCs deliver ~2.2−3.9 mW cm^{-2} regardless of the fuels, allowing choosing the fuel due to availability. The benchmark of 6.76 mW cm^{-2} was found using ethylene glycol [3]. To decrease the price of a disposable paper battery, we used 5 to 90 s sputtering Pt on a CP, to produce an atomic resolution and very low content Pt/CP. In an unpublished work, using the 60 s sputtered CP and a metal-free cathode ethylene glycol paper battery, we found > 9 mW cm^{-2} as the maximum power density, which is the benchmark for similar devices. We also have been investigating paper-batteries fed by glucose, aiming further application using biological fluids. Working with Pt/C/CP anode and CP cathode, we already found the dependence of the output power with the glucose concentration. The anode seems to experience self-poisoning, delivering a maximum of >2,3 mW cm^{-2} when fed by glucose 0.1 mol L^{-1}. I hope this talk encourages researchers to explore new paper-based energy converters based eco-friendly fuels.

References

[1] O.A. Ibrahim, M. Navarro-Segarra, P. Sadeghi, N. Sabaté, J.P. Esquivel, E. Kjeang, Microfluidics for Electrochemical Energy Conversion, Chem. Rev. (2022). https://doi.org/10.1021/acs.chemrev.1c00499.
[2] I.L. Vera-Estrada, J.M. Olivares-Ramírez, J. Rodríguez-Reséndiz, A. Dector, J.D. Mendiola-Santibañez, D.M. Amaya-Cruz, A. Sosa-Domínguez, D. Ortega-Díaz, D. Dector, V.M. Ovando-Medina, I.D. Antonio-Carmona, Digital Pregnancy Test Powered by an Air-Breathing Paper-Based Microfluidic Fuel Cell Stack Using Human Urine as Fuel, Sensors. 22 (2022) 6641. https://doi.org/10.3390/s22176641.
[3] A.L.D. Lima, P.M. Rocha, A.C. Silva, J. Alves Fernandes, C.A. Martins, Interchangeable Biomass Fuels for Paper-Based Microfluidic Fuel Cells: Finding Their Power Density Limits, ACS Appl. Mater. Interfaces. 15 (2023) 11895–11905. https://doi.org/10.1021/acsami.2c23192.

I17. Development of biocompatible thin piezoelectric films for various applications

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Recently, the focus of research has turned to biomolecular piezoelectrics with sufficiently high piezoelectric properties and intrinsic compatibility with the biological environment. It is based on the complex dipolar properties and dipole-dipole interactions conjugated with hydrogen bonds network in biomolecular systems with different levels of self-assembly and hierarchy. Piezoelectricity in biological objects was found in a number of biological materials of different natures. It is inevitable that such a high coupling will be present in more simple bioorganic materials such as amino acids and peptides. However, only recently emergent piezoelectric properties ($d24 \approx 190$ pm/V) have been discovered in crystalline glycine [1]. The voltage piezoelectric coefficient (needed for biomedical applications is 8 V/mN, i.e. several orders of magnitude higher than in the previously used P(VDF-TrFE)]. Recent investigations show that this material can be prepared and stabilized in a thin film form and it is full of ferroelectric domains that can be used as movable conducting interfaces.

Strong piezoelectricity has been discovered in bio-inspired nanotubes made by a self-assembly process of diphenylalanine monomers [2]. These peptide nanotubes (PNTs) originate from the smallest recognition motif of the amyloid-Aβ protein, associated with over 30 neurodegenerative diseases, such as Alzheimer's, Parkinson's, etc. They are made of amino acids, which are self-assembled in unique stable tubes with hydrophilic hollows, having high Young's modulus and profound chemical stability. Recent efforts of our team from University of Aveiro have focused on understanding the strong piezoelectric properties of peptide nanostructures, prototyping, and optimizing growth conditions [3, 4]. A major problem is an inability to control the self-assembly process to produce dense films with controlled orientation and thickness. To overcome this, we propose a novel method of the formation of crystalline piezoactive FF films via solid phase crystallization directly from the amorphous phase [5]. The process starts with the spin-coating of FF monomers in an organic solution. These layers are then exposed to a controlled humidity that triggers nucleation and growth of highly oriented piezoactive areas (domains). The crystallization process proceeds without changing the morphology and results in dense films with controlled thickness. Large ferroelectric-like domains possess uniform piezoresponse of about 30 pm/V with the in-plane polarization. The growth kinetics is controlled by the temperature and humidity, suggesting that fully in-plane oriented films can be obtained. This is a promising result for the development of multifunctional devices to meet various application requirements, which is an important development trend nowadays.

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1. S. Guerin, A. Stapleton, D. Chovan, et al. “Supramolecular packing controls piezoelectricity in amino acids”, Nature Mater. 17, 180 (2018)
2. A. Kholkin, N. Amdursky, I. Bdikin, E. Gazit, and G. Rosenman, “Strong piezoelectricity in bioinspired peptide nanotubes”, ACS Nano 4 (2), 610-614 (2010)
3. E. Bosne, A. Heredia, S. Kopyl, D. V. Karpinsky, A. G. Pinto, and A. L. Kholkin, “Piezoelectric resonators based on self-assembled diphenylalanine microtubes” Appl. Phys. Lett. 102 (7), 073504 (2013)
4. P.S. Zelenovskii, K. Romanyuk, M. S. Liberato et al, “2D layered dipeptide crystals for piezoelectric applications”, Adv. Funct. Mater. 31, 43 (2021)
5. K. Romanyuk, V. Slabov, D. Alikin,et al “Piezoactive dense diphenylalanine thin films via solid-phase crystallization”, Appl. Mater. Today. 26, 101261 (2022).

I18. Nanofiber-Based Hydrogels for Drug Delivery Systems

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Abstract

Hydrogel drug delivery systems, which are in the field of drug delivery systems in the biomedical field, are attracting increasing interest from researchers around the world. Electrospinning technique is a technique that allows the loading of a higher concentration of therapeutic agents per unit mass of a polymer, thus providing encapsulation of the drug within the fiber, providing protection and long-term drug release. In this study, drug-loaded nanofiber hydrogels were successfully produced by electrospinning process.

Introduction

Drug delivery systems are one of the current topics in the field of biomedicine, which can make the administration of drugs more effective, safe and convenient [1]. Hydrogels have found extensive applications in various medical fields, including drug delivery and wound dressing, due to their biocompatibility, biodegradability, and high water uptake [2]. Despite their unique properties, the application of hydrogels is limited by their low surface-to-volume ratio and poor mechanical properties. On the other hand, nanofibers have found increasing popularity due to their high aspect ratio, favorable strength, excellent mechanical properties and easy processing [3]. Electrospinning has become an attractive technique in biomedical research, especially in tissue engineering, thanks to the ability to adjust the properties of nanofibers and the fact that it is a simple method in which various polymers can be used cost-effectively [4].

Method

Gentamicin (Gent), an antibiotic, was used. Nanofiber-Based Hydrogels were produced by the electrospinning method using a double-pump electrospinning device. It was prepared by mixing polymeric solutions with Gent solutions in certain proportions (between 5-10% by weight compared to the polymer content) until they become homogeneous. The prepared polymeric solutions were kept in vacuum for 6 s to remove air bubbles. Each solution was loaded into a 1 mL syringe containing a stainless steel syringe needle. The flow rate was controlled by a pump and the flow rate was set in mL/s to ensure uninterrupted solution jetting. A high electrical voltage was applied, which would be predetermined by the high voltage source to provide a sufficient electric field for electrospinning. After the optimization step of the distance between the needle and the collector, a rotating drum wrapped with aluminum foil was used to collect polymeric nanofiber hydrogels. The produced polymeric hydrogel nanofibers were stored at 4°C.

Results and Discussion

As can be seen in Figure 1, Nanofiber-Based Hydrogels were prepared successfully. The use of a cylindrical collector instead of a flat plate in the electrospinning system resulted in a more regular fiber structure. Nanofiber-Based Hydrogels with different morphologies were created thanks to variables such as the polymer solution used, voltage, feeding speed of the syringe, and the distance between the needle and the collector.

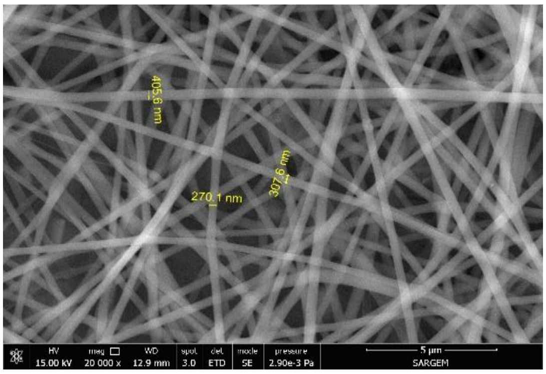

Figure 1. Nanofiber-Based Hydrogels samples produced by electrospinning system.

Conclusion

The large surface area and porous structure of the nanofiber membrane can be effectively loaded with various biologically active ingredients, including antibacterial drugs, inorganic nanoparticles, vitamins, growth factors, and plant extracts. The drug release rate and duration could be controlled by adjusting the fiber structure and morphological size.

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References

[1] S. Hajebi, N. Rabiee, M. Bagherzadeh, S. Ahmadi, M. Rabiee, H. Roghani-Mamaqani, M. Tahriri, L. Tayebi, M.R. Hamblin, Stimulus-responsive polymeric nanogels as smart drug delivery systems, Acta Biomater., **92**, 1–18 (2019).
[2] R. Tutar, A. Motealleh, A. Khademhosseini, N.S. Kehr, Functional Nanomaterials on 2D Surfaces and in 3D Nanocomposite Hydrogels for Biomedical Applications, Adv. Funct. Mater. **29**, 1–29, (2019).
[3] A. Chyzy, M. Tomczykowa, M.E. Plonska-Brzezinska, Hydrogels as potential nano-, micro- and macro-scale systems for controlled drug delivery, Materials (Basel). **13**, 188, (2020).
[4] Z. Mohammadalizadeh, E. Bahremandi-Toloue, S. Karbasi, Recent advances in modification strategies of pre- and post-electrospinning of nanofiber scaffolds in tissue engineering, React. Funct. Polym. **172**, 105202, (2022).

I19. Carbon nanotube-enabled scaffolds: fabrication, characterization, in vitro studies, nanotoxicology and prospects

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Significant research efforts have been made to exploit carbon nanotubes (CNTs) as nanotransducers to enhance and modulate cell biological activities, some of them with great success. However, the safety concerns associated with the possible short- and long-term toxicity of CNTs is still holding back their transferability from research to clinical trials of such devices. Here, we present different strategies of the use of CNTs for cell modulation, including pseudo-3D templates and electromagnetic-responsive CNT-enabled (rigid and injectable) scaffolds. The CNT pseudo-3D templates have supported long-term survival of the cells in comparison to the control templates and modulated cell orientation along any created patterns (such as spirals and stripes). These templates could be used to create in vitro platforms for fundamental studies of cell behavior. Electromagnetic-responsive CNTs were synthesized and integrated into collagen/PLA scaffolds. A comprehensive in vitro study using chondrocytes showed that CNT-enabled scaffolds boost cell metabolic activity while maintaining cell viability and extracellular matrix expression. No significant effects were observed on the cell response due to the applied external magnetic stimuli. A reproducible method to remotely align CNTs into injectable hydrogels using magnetic field was also successfully achieved. In addition, in vitro safety assessment performed for the synthesized CNTs and as well CNT-enabled collagen/PLA scaffolds are presented here. The results provide evidence supporting the claim that CNTs are generally safe as part of a composite biomaterial. The prospects of CNT use in implantable medical devices will be briefly presented, aiming to open discussions regarding the regulatory aspects of the safe use of CNT-enabled devices.

I20. Ammonia for decarbonizing our world?

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A principal aim of the EU 2030 climate & energy framework is the reduction of CO_2 emissions by developing new technologies for industries and processes [1]. There is an urgent need for a transition to a green economy, where the fabrication of sustainable chemicals is deeply urged [2]. In this regard, ammonia (NH_3) is a key chemical produced in vast quantities worldwide as a precursor in a range of products vital to society, such as fertilizers and medicines. Nonetheless, its current industrial production (Haber-Bosch method) requires high temperatures and pressures, producing large quantities of CO_2 due to its continued reliance on H_2 from natural gas [3]. In this regard, the electrochemical synthesis of NH_3 using a Proton Ceramic Electrochemical Cell (PCEC) is a highly attractive alternative to mitigate this problem, where this compound can be directly synthesized from renewable sources with minimum pollution. This technology offers a highly promising and potentially disruptive route to synthesize one of the most important chemicals extensively used worldwide.

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References
[1] “EU 2030 climate & energy framework”, https://www.un.org/sustainabledevelopment/sustainable-development-goals/.
[2] “EU iea report: Chemicals”, https://www.iea.org/reports/chemicals.
[3] Kyriakou V, Garagounis I, Vasileiou E, Vourros A, Stoukides M. "Progress in the Electrochemical Synthesis of Ammonia", Catal Today, vol. 286, pp. 2-13, 2017.

I21. Photocatalytic performance of Rare-earth orthchromite-reduced graphene oxide nanocomposites for wastewater treatment

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DyCrO3/r-GO (DCO/r-GO) and Dy0.5Ho0.5CrO3/r-GO (DHCO/r-GO) nanocomposites consisting of 5 wt.% r-GO were synthesized by the sol-gel method and their photocatalytic performance was studied on methylene blue (MB) and rhodamine B (RhB) dyes under solar irradiation. The bandgap energy of DCO/r-GO and DHCO/r-GO nanocomposites was found to be 2.63 eV and 2.58 eV, respectively. The DCO/r-GO and DHCO/r-GO nanocomposites demonstrated remarkably higher photocatalytic activity (PCA) than DCO and DHCO nanoparticles. The DCO/r-GO and DHCO/r-GO nanocomposites furnished 69.6% and 71.6% degradation of the MB dye and 87% and 96% degradation of RhB dye within 180 min under direct sunlight.

I22. Analogous environment study of the Naica mine (dehydrated calcium sulfate $CaSO4 \cdot 2H2O$): A DFT approach to molecular dynamics

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The Naica Caves in Chihuahua Mexico have been the subject of various studies due to their composition, large-sized crystals, and extreme environments. The largest crystals found in these caves are selenite ($CaSO4 \cdot 2H2O$), which are formed due to high concentrations of sulfur, oxygen, and metallic cations. These components precipitate as anhydrite ($CaSO4$) at temperatures below 58°C, and with a decrease in temperature, they hydrate to become selenite at the end of the process. This leads us to emphasize the behavior of selenite at temperatures higher than ambient in order to understand the anomaly of its dimensions and its interaction with organic compounds that could be remnants of life. Therefore, the objective of this work is to implement the molecular dynamics theory using the plane-wave pseudopotential method through the CASTEP code to run a temperature ramp on the bulk structure of the mineral and observe possible conformational changes, similar to experiments in Differential Scanning Calorimetry. In both cases, the Perdew-Burke-Ernzerhof (PBE) functional was employed based on the results obtained in the optimization process. The NVT ensemble was used with a Nosé-Hoover thermostat, and the system temperature was varied between 25 and 150°C. The simulation was performed with a time step of 1 fs and total simulation times of 1 fs, 100 fs, and 500 fs. The results show the evolution of the lattice parameters (length, angles, and volume) as the system temperature increases. Finally, the computational results obtained in this work will serve as a guide, at the nanoscale, to understand the relevance of selforganization and prebiotic catalysis of organic compounds in TGA and DSC experiments.

L.S.N. and U.L.P. appreciate the support of the PAPIIT-UNAM projects IN110919 and IN205522. C.M.F. thanks the support of DGAPA-UNAM for the postdoctoral scholarship. We appreciate the support of Luciano Diaz and Eduardo Murrieta for the maintenance and operation of the ICN-UNAM computer equipment.

I23. Contribution of nanoscale calorimetry to material characterization

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This talk will give an overview of what can be investigated through a recent device: The Fast Scanning Calorimetry (FSC). FSC has recently emerged as a very powerful calorimetric technique, allowing to analyze few nanograms of material, and to characterize the microstructure under very high scanning rate covering more or less seven decades.

Among results obtained thanks to FSC, some refer to topics such as crystallization kinetics in polymeric systems, crystalline reorganization, nucleation in metallic alloys, etc. This talk will present recent results obtained by the authors [1-5]. A focus will be done on works related to the characterization of the physical aging process [3-5]. Indeed, the FSC offers the possibility to accelerate this natural process, which can occur on one-hundred-year timescale, and thus to analyze it in the laboratory timescale [6].

References:

[1] X. Monnier, J.E. Maigret, D. Lourdin, A. Saiter. *Carbohydrate Polymers*, **173,** 77 (2017).
[2] B. Atawa, N. Couvrat, G. Coquerel, E. Dargent, A. Saiter. *International Journal of Pharmaceutics*, **540**, 11 (2018).
[3] X. Monnier, N. Delpouve, A. Saiter-Fourcin. *Soft Matter,* **16**, 3224 (2020).
[4] A. Morvan, N. Delpouve, A. Vella, A. Saiter-Fourcin. *Journal of Non-Crystalline Solids,* **570,** 121013 (2021).
[5] A. Morvan, L. Calvez, A. Vella, A. Saiter-Fourcin, *Journal of Non-Crystalline Solids* **598**, 121955 (2022).
[6] X. Monnier, A. Saiter, E. Dargent. *Thermochimica Acta*, **648**, 13 (2017).

I24. Dimensionally modified structures for caloric applications: an experimental study

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To reduce greenhouse gas emissions caused by the current vapor-compression-based cooling technology, it is necessary to design low-noise and environmentally friendly refrigerants. Electric field-induced cooling can be viewed in this light as a promising, fast and affordable on-chip cooling method that can be scaled down to smaller dimensions. Nanostructures with switchable polarization, and near phase transitions, can exhibit large entropy changes that can be tuned by tailoring material properties[1,2]. Compared to bulk crystals, artificially engineered ferroelectric heterostructures such as epitaxial thin films, possess inherent advantages for easy integration in microelectronics with higher efficiency energy-recovery strategies.

In the current work, we developed and investigated caloric effects of two different oxide materials (binary and perovskite) with varied dimensions. Detailed structure/microstructure and physical properties were evaluated. In-depth x-ray diffraction studies confirmed oriented growth of oxide ferroelectrics with varied lattice strains. In addition, binary oxide materials with different doping concentrations exhibited negative and positive caloric properties due to compositional changes. We observed adiabtic temperature changes >10 K and 6 K respectively for perovskite and binary oxide nanostructures. The results suggest that the growth of high-quality nanostructures with tuned lattice strain and dimensions are great candidates for future echo-friendly refrigerants that operate at moderate external stimuli for energy-efficient solid-state cooling.

References

[1] E. Venkata Ramana et al., Surfaces and Interfaces 33, 102257 (2022) 102257.
[2] E. Venkata Ramana et al., Journal of the European Ceramic Society 41 (2021) 6424–6440.

I25. Innovation in Chemical and Electrochemical Treatment and Recovery of Precious Metals

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Precious metals (PMs) are non-renewable in nature, but the demand and consumption increase continuously. It turns more and more attention to the recovery of gold, Pt-group metals (PGMs) from secondary resources such as waste of electric and electronic equipment (WEEE) and waste of spent catalysts (WSC). Hydrometallurgy is a widely used process for PMs leaching and recovery; it involves several chemical reactions in liquid media. The first step of each hydrometallurgical recycling technique is leaching of PMs to the some liquid media. The biggest enterprises acting in metals recycling industry the leaching carry out in the aqua regia: HCl, HNO_3, H_2SO_4, cyanide, etc., i.e. consuming cheap, but aggressive and toxic chemicals. However, the WEEE and WSA are collected in each country, and the demand to recovery Au, PGMs on local enterprises using non-toxic and less aggressive constituents in profitable way is growing up.

In the meantime, researchers have continuously improved the PMs leaching and recovery strategies that are based on the mechanism of the aqua regia method, in particular using various ligands in order to dissolve PMs: concentrated chlorides, thiosulfates, thiourea, ammonia. As concentration of PMs from diluted solutions, the selective adsorption techniques are investigated.

In addition, recovery of leached metal via electrowinning technique is one of the alternative ways for desired metal recovery. This technique can be used for electrowinning of based metals. As a case study the perspectives of tin electrowinning from citrate-based solutions is assessed.

Acknowledgement: This research has received funding from Horizon 2020 research and innovation program under MSCA-RISE-2017 (No. 778357).

I26. Behind the enhanced electrical performance of Flash sintered potassium sodium niobate ceramics

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In view of sensor, actuator, and energy harvesting applications, lead-free $K_{0.5}Na_{0.5}NbO_3$ (KNN) ceramics present such benefits as high ferroelectric transition temperature and elevated piezoelectric coefficient, if their content of secondary phases is diminished. Alternative sintering techniques, including electric field- and current-assisted Flash sintering, are promising for low thermal budget production of single-phase KNN ceramics, which electrical properties however have not been widely disclosed so far. Here, KNN ceramics Flash sintered at 900 ºC for 60 s only is successfully demonstrated to be of high performance. These ceramics with Pt electrodes cured at 900 ºC possess room-temperature remnant polarization P_r = 21 µC/cm^2 and longitudinal piezoelectric coefficient d_{33} = 117 pC/N, slightly superior to that for KNN ceramics conventionally sintered at 1125 ºC for 3 h with identical electrodes [1]. At the same time, the electrical performance of as-sintered ceramics obtained using Flash and conventional processes with sputtered Au electrodes has opposite relation. Thus, comparative and systematic ferroelectric, dielectric permittivity, impedance spectroscopy, and DC conductivity analysis shows that heat treatment, synergistically needed for the Pt electrode curing and ceramic defect relaxation, is not less important than the low thermal budget Flash sintering process for potential applications of Flash KNN ceramics in innovative low-carbon technologies.

References

[1] R. Serrazina, A. Tkach, L. Pereira, A.M.O.R. Senos, P.M. Vilarinho, *Materials*, **15**, 6603 (2022).

I27. Towards Chromium (VI) Replacement: Combination of Electrochemical Deposition and PVD Coatings

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The European union REACH Regulation (EC) No 1907/2006 (annex XIV) has included chromium trioxide or hexavalent chromium as a substance of very high concern. Consequently, the use of hexavalent chromium requires its progressive replacement by a proper substance and/or technology. The most analysed technology to use as an alternative to hexavalent chromium is electroplating using solutions containing trivalent chromium. Other technologies such as PVD, nickel electro/electroless plating, and thermal spraying are also alternative candidates to replace hexavalent chromium. The most promising substitutes to hexavalent chromium coatings and analysis of the industrial transition from hexavalent chromium coatings towards more sustainable alternatives are briefly reviewed in this work. Preliminary results concerning electrochemical deposition followed by PVD coatings demonstrate the viability of such option within the industrial sector for decorative purposes. Nonetheless, numerous improvements are still necessary to attain the compulsory chromium (VI) replacement by the combination of both technologies.

I28. Improving sample classification for photodiagnosis

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The identification of multidrug-resistant strains of E. coli responsible for calf diarrhea still faces several laboratory challenges but is essential for effective monitoring and control of this microorganism's spread. To address this, there is a pressing need to develop a user-friendly, rapid, and accurate screening tool for bacterial strain identification in microbiology laboratories. In this context, the utilization of FTIR spectroscopy for microorganism identification has been well-established in the scientific literature, encompassing various bacterial strains. In this study, we aimed to harness the potential of FTIR for identifying multidrug-resistant E. coli strains. Our approach began with principal component analysis to assess any grouping tendencies. Initially, the results displayed a scattered sample score distribution with no clear clustering. However, by carefully selecting the key principal components contributing to group separation, we enhanced the clarity of our findings. Ultimately, by employing machine learning algorithms, our predictive model achieved an impressive 70% overall accuracy, underlining the method's suitability as a screening tool for microorganism identification."

References

[1] B.S> Rezende, T. Franca, M.A.B. Paula, H.P.K. Cleveland, C. Cena, C.A.N. Ramos, Turning chaotic sample group clusterization into organized ones by feature selection: Application on photodiagnosis of Brucella abortus serological test, Journal of Photochemistry and Photobiology (2023).
[2] Y.G. Marangoni, T. Franca, J. Esteves, A. Maranni, K.D.O Portes, C. Leal, C. Cena. Multi-resistant diarrheagenic Escherichia coli identified by FTIR and machine learning: a feasible strategy to improve the group classification, RSC Advances (2023).
[3] T.G. Rios, G. Larios, B. Marangoni, S.L. Oliveira, C. Cena, C.A.N. Ramos, FTIR spectroscopy with machine learning: A new approach to animal DNA polymorphism screening, Spectrochimica Acta A (2021)

I29. Analogy of different optical temperature sensing techniques in rare earth doped materials

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Temperature is one of the important thermodynamic parameters that plays a crucial role in various areas of science and technology. Accurately measuring temperature in a variety of environments can be a difficult task due to physical, chemical, and biological limitations. At present, commonly used devices are thermometers, thermistors, thermometers, thermocouples, and thermal paints. All requires, direct object contact, which impose constrains in invasive environments like harsh, corrosive and bio environments. Nevertheless, the demand for precise temperature measurements remains essential. Alternatively, optical thermometry allowing detection in inaccessible environments with high accuracy and fast response speed. The effects of temperature on various luminescent properties, including spectral shifts, bandwidth changes, intensity variations, and polarization modifications, are examined as reliable indicators for temperature assessment. Optical thermometry based on Upconversion/Downconversion luminescence has been extensively studied because of its exceptional advantages, such as large-scale imaging, contactless measurement, and others. This presentation discusses a novel approach to temperature sensing via rare earth photoluminescence. Three of the possible approaches to optical temperature sensing of a thermographic phosphor were formally compared and discussed rare-earth doped phosphors. Namely fluorescence intensity ratio (FIR) of thermally coupled levels (TCL), Valley to Peak ratio (VPR) and the ratio of non-thermally coupled levels (NTCL).

References

[1] K. Pavani etal., *Ceramics International*, **48**, 31344-31353 (2022).
[2] K. Pavani etal., *White Light Emitting Upconversion Nanomaterials*, Springer, 2023.
[3] K. Pavani etal., Journal of Luminescence, 235, 117992

Oral presentations

O1. Interaction Mechanisms of Gold, Silver, and Copper Nanoparticles protected by Cysteine: optical properties, environmental applications and biocompatibility

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Cysteine-protected metal NPs (MetalCys NPs) have shown interesting optical properties, water-solubility for environmental applications, and bio-compatibility for biomedical applications, and they have been central subject for the study of protein interactions with NPs as bioconjugates and protein folding. Herein, cysteine interaction with gold, silver, and copper NPs is characterized by Raman spectroscopy and density functional theory calculations to elucidate the molecular conformation and adsorption sites for each metal. The experimental analysis of Raman spectra upon adsorption with respect to free cysteine indicates that while the C−S bond and carboxyl group are similarly affected by adsorption on the three metal NPs, the amino group is sterically influenced by the electronegativity of each metal, causing a greater modification in the case of gold NPs. A theoretical approach that takes into consideration intermolecular interactions using two cysteine molecules is proposed using a S−metal−S interface motif anchored to the metal surface. These interactions generate the stabilization of an organo−metallic complex that combines gauche (PH) and anti (PC) rotameric conformers of cysteine on the surface of all three metals that also confirms the thiol and carboxyl groups as adsorption groups for gold, silver, and copper NPs.

References

[1] Pan, M.; Yang, J.; Liu, K.; Yin, Z.; Ma, T.; Liu, S.; Xu, L.; Wang, S. Nanomaterials 2020, 10, 209.
[2] Gao, X.; Zhuang, X.; Tian, C.; Liu, H.; Lai, W.-F.; Wang, Z.; Yang, X.; Chen, L.; Rogach, A. L. Sens. Actuators, B 2020, 307, 127626.
[3] Anand, S. K.; Mathew, M. R.; Kumar, K. G. J. Fluoresc. 2019, 30, 63−70.

O2. Investigation of mechanical properties in new 2D-structure Irida-Graphene by using molecular dynamics simulation

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The design [1] and synthesis [2] of new carbon allotropes have experienced enormous growth since the advent of graphene. In this study, the mechanical properties of a new carbon allotrope called Irida-Graphene is investigated by LAMMPS package. This new 2D all-sp^2 carbon allotrope composed of 3-6-8 rings named Irida-Graphene [3]. This name is due to its atomic arrangement that resembles the flower in the United States. The AIREBO interatomic potential was used to describe the interactions between the C-C bonds. The temperature of Irida-Graphene was controlled by Nose-Hoover thermostat in canonical ensemble. The effect of temperature on the stress-strain diagram as well as mechanical properties are investigated. We observed that Young's modulus, fracture strain and strength are totally dependent on simulation's temperature and they decreased sharply by increasing the temperature. Moreover, our molecular dynamics simulation shows effect of temperature on the stress-strain diagram of Irida-Graphene.

References

[1] L. Yang, H.Y. He, B.C. Pan, Theoretical prediction of new carbon allotropes, J. Chem. Phys. 138 (2) (2013), 024502.

[2] Chee-Tat Toh, Hongji Zhang, Junhao Lin, Alexander S Mayorov, Yun-Peng Wang, Carlo M Orofeo, Darim Badur Ferry, Henrik Andersen, Nurbek Kakenov, Zenglong Guo, et al., Synthesis and properties of free-standing monolayer amorphous carbon, Nature 577 (7789) (2020) 199–203.

[3] Júnior, ML Pereira, et al. "Irida-graphene: A new 2d carbon allotrope." *FlatChem* 37 (2023): 100469.

O3. Cyclometallated Iridium Complexes containing ppy type ligands

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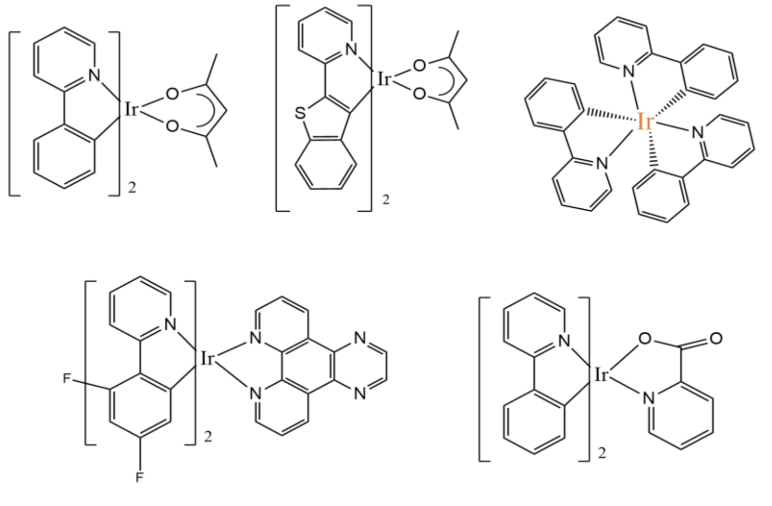
Iridium complexes have drawn attraction due to potential application in various fields Cyclometalated. Iridium complex have been widely synthesised and screened for various properties in recent years. They have been widely used as chemosensors, photooxidants, photocatalysts, sensitizers, bioimaging and anticancer drugs etc.

Phosphorescent iridium (III) complexes have been commonly used as light emitting material in common Organic light-emitting diodes (OLEDs) due to their high quantum efficiency. [1]They show various range of tunable light emission by different type of attached ligands.[2] The strong spin–orbit coupling induced fast intersystem crossing (ISC) causes iridium complex as luminescence materials. Phosphorescence emission is caused by mixed excited triplet states i.e. LC and MLCT. Now a days it has become a challenging task to bring quantum efficiency to unit at room temperature in the field of inorganic photochemistry.So far iridium complexes having 12.3% external quantum efficiencies have been reported by some groups.



Some cyclometalated luminescence Iridium complexes

References:

[1] Adachi, C.; Baldo, M. A.; Forrest, S. R.; Thompson, M. E. *Appl. Phys. Lett.* **2000**, *77*, 6904.

[2] Lee KH, Kang HJ, Kim SO, Lee SJ, Seo JH, Kim YK, Yoon SS , Mol. Cryst.Liq. Cryst., 2010, 530,186–195

O4. Interaction between cerium and oxygen films on Mo(112): surface structure and electronic properties

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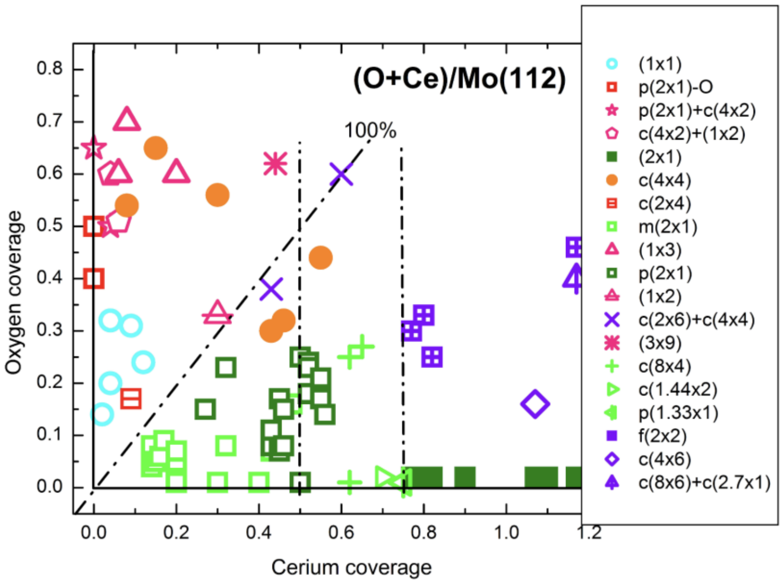
Studies of oxygen interaction with metal adatoms are important for many applied materials science areas such as corrosion protection, catalysis, hydrogen energy materials, electronics, and medicine. At the same time, the metal-oxygen system is an interesting model for research of fundamental aspects of the atomic interactions (due to the relatively high electronegativity of oxygen atoms) and there are numerous phenomena that have been reported for such systems. [1,2]

In this research, we studied the coadsorption of cerium and oxygen films in wide coverage ranges: $\theta_{Ce} = 0 - 1.2$, $\theta_o = 0 - 0.8$. Surface structure, composition and work function of the system have been measured by low energy electron diffraction (LEED), Auger electron spectroscopy (AES) and contact potential difference (CPD) in ultrahigh vacuum (UHV) conditions.

The presence of various surface structures at room temperature (RT) in dependence on the Ce and O coverages is shown on a diagram (fig.1):



The possibility of oxides formation and the nature of the atoms' interaction have been discussed based on the observed structures and work function changes.

References

[1] K. Budde, L. Schwenger, C. Voges, and H. Pfnür, *Phys. Rev. B,* **52**, 9275 (1995).
[2] G. Godzik, T. Block, and H. Pfnür, *Phys. Rev. B,* **69,** 235414 (2004).

O5. Investigation and effect of $CeVO_4$/TiO_2/SnS composite on synthesis and oxygen evaluation reactions (OER)

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- Abstract

In this study, a ternary nanocomposite $CeVO_4$/TiO_2/SnS photoelectrode was synthesized by hydrothermal method and its effects on the photoelectrochemical water splitting reaction were investigated. Then, XRD and SEM characterizations of the synthesized nanoparticles were carried out. These synthesized samples were coated on ITO glass and their OER capacities were determined under 150W halogen lamp. The OER capacity of prepared ternary composites was evaluated by using I-V and Tafel curves. The results obtained show that the ternary composite has a synergistic effect with the increase in oxygen production compared to pristine semiconductor.

- Introduction

While the need for energy in the world continues to increase last years, efforts for the usage of renewable energy sources have gained great importance in order to meet this increasing need due to the rapid depletion of fossil fuels and environmental problems [1]. Hydrogen energy is the most remarkable energy among renewable energy sources. Due to the costs of storing hydrogen, different production techniques of hydrogen are being developed. Therefore, studies on alternative hydrogen production methods and systems have gained momentum in recent years. Among them, photoelectrochemical production of both H_2 and O_2 from water is both environmentally friendly and an innovative approach [2].

- Method

Synthesis and characterization of $CeVO_4$, TiO_2 and SnS nanostructures

5mmol $Ce(NO_3)_3.6H_2O$ and 5mmol NH_4VO_3 were resolved in 40 mL of ultra-pure water (UPW) and mixed in a magnetic mixer for 30 min. 1M NaOH was supplemented until the pH of the solution was 10-12. 5 mL titanium isopropoxide (TTIP) was supplemented dropwise to 40 mL UPW including 5 mL 1 M NaOH solution and mixed 30 min. 1.6 mmol $SnCl_2{\cdot}H_2O$, 80 µL thioglycolic acid (TGA) and 80 mM 160 mL Na_2S solution were mixed in a beaker for 10 min. Then each mixture were taken to separately Teflon-based hydrothermal containers and subjected to, 18 h for $CeVO_4$, 15 h for TiO_2 and 15 h for SnS heat treatment at 180°C. The synthesized all nanostructures were separated via centrifuge and washed three times with UPW and 2 times with ethanol and dried overnight at 80°C. Synthesized all nanostructures were characterized via XRD and FESEM.

Photoelectrochemical O_2 evaluation

The photoelectrode was prepared via drop casting on ITO substrates. ITO substrate was cleaned in UPW, acetone, ethanol/water (1:1) mixture and 0.1 M NaOH solution via sonication, respectively. Then, separately, 4 mg/L $CeVO_4$, 4 mg/L TiO_2 and 4 mg/L SnS were dispersed in methanol and vigorously stirred 30 min to homogenization. 4-µL SnS, 4-µL TiO_2 and 4-µL $CeVO_4$ were coated dropwise on the ITO substrate, respectively. The resulting photoelectrode dried under room conditions and was reserved in the dark. Photoelectrochemical water decomposition reactions were studied by linear sweep voltammetry (LSV) technique in 1 M Na_2SO_3, 1 M NaOH or 1 M H_2SO_4 environments under 100 W halogen lamp using a conventional electrochemical cell consisting of Pt wire counter electrode, Ag/AgCl reference electrode and prepared working photoelectrodes. In addition, the H_2 and O_2 production efficiencies were investigated by taking electrochemical impedance curves and Tafel curves for the purpose of studying conductivity behavior.

- Results

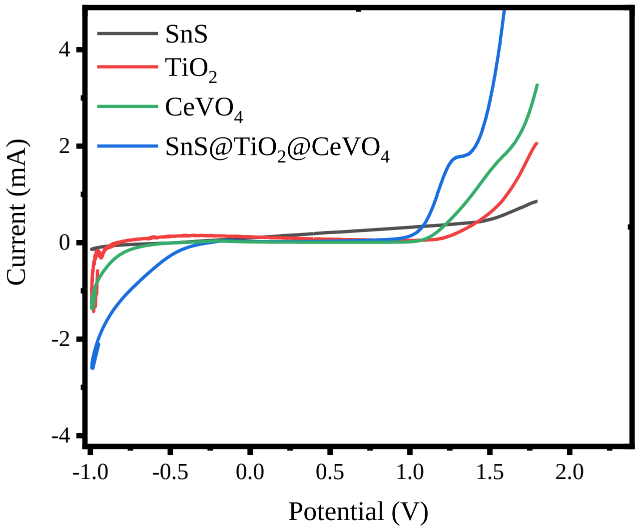

Fig. 1. The LSV curves of the synthesized nanostructures

The LSV results of photoelectrodes prepared with synthesized SnS and TiO_2 and $CeVO_4$ samples are shown in Fig. 1, respectively.
In these synthesized nanostructures, a sudden increase in current values over 1.0 V was observed depending on the voltage increase. In addition, the sensitivity of these synthesized structures to light was proven by the increase in current under light. The voltage potentials of the nanostructures correspond to 900 mV, 700-1000 mV, 900-1300 mV for SnS and TiO_2 and $CeVO_4$, respectively.

- Discussion

In this study, semiconductor photoanodes with different properties, which adopt the basic principles of photoelectrochemical water separation, are synthesized and their effect to water splitting under visible light were investigated. The band gaps of the semiconductor materials used for photoelectrochemical water splitting should be compatible with the reduction and oxidation potential of water. They must also contain suitable load carriers for OER to occur. The $SnS/TiO_2/CeVO_4$ ternary composite electrode prepared in this study caused higher photocurrent generation and faster recombination compared to pristine semiconductors. Metal nanoparticles (esp. noble metal) doping method can be applied to increase the photocurrent values of these synthesized composite photoanodes under visible light.

References

[1] E.L. Miller, Energy Environ. Sci. 8, 2809–2810 (2015). https://doi.org/10.1039/c5ee90047f.

[2] A. Eftekhari, V.J. Babu, S. Ramakrishna, Int. J. Hydrogen Energy 42 11078–11109, (2017). https://doi.org/10.1016/j.ijhydene.2017.03.029.

O6. The ITO/rGO@SnS@CeVO$_4$ nanocomposite photoanode for a photosensitive detection of Tyrosine

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Abstract

Tyrosine is required for the production of certain neurotransmitters (chemicals important to the brain) such as dopamine, epinephrine, and norepinephrine, and is a non-essential amino acid that the body synthesizes from another amino acid (phenylalanine). In current study, a photo-sensitive ITO/rGO@SnS@CeVO$_4$ based sensor is fabricated for Tyrosine detection. Tyrosine is analysed by photo-sensitive ITO/rGO@SnS@CeVO$_4$ sensor at solutions posses diverse concentrations in 0.1 M PBS environment. The Tyrosine sensor worked in the 1-75 µM linear range. Our study can help to improve novel photosensitive amino acid sensors.

Introduction

Amino acids are the smallest units that make up proteins, and have essential roles in organisms such as proteins, hormones and neurotransmitters that are vital in the living body. They are also found in the structure of hormones and enzymes, and they are together in the cell membrane thanks to lipids [1]. It is an organic ring with amine (-NH$_3^+$), carboxyl (-COOH) and side chain ® groups in its structure. Amino acids have a total of 20 members consisting of two different groups, essential such as lysine, leucine, phenylalanine, tryptophan etc., and non-essential amino acids like glycine, cysteine, alanine, tyrosine etc. [2].

- Method

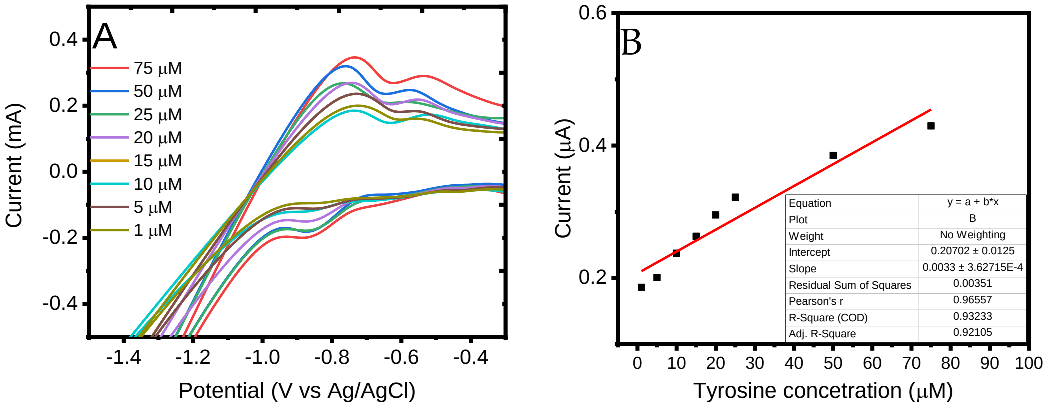
1- rGO synthesis and characterizations

Hummers method, which is widely used in the literature, was used for rGO synthesis. 16 mL of concentrated H_2SO_4, 5 g of $KmnO_4$ and 6 g of $NaNO_3$ were supplemented to 10 g of graphite, it was refluxed at 80oC for 2 h. This solution was then cooled at room temperature overnight and kept in the dark. This solution was washed several times with distilled water until it reached neutral pH. In order to complete the oxidation of this partially oxidized graphite, it was slowly added with 34 g of $KmnO_4$ and 240 mL of H_2SO_4 in an ice bath at 0^{o}C. The temperature of this mixture was constantly controlled to ensure that it did not rise above 20^{o}C. Then, 1L distilled water was added to this mixture and refluxed at 35^{o}C for 2 h. Then, the reduction was carried out by adding 20 mL of H_2O_2 to the solution. This mixture was purified from metals and impurities by washing with 1:10 HCl solution (1L). Then, the dark brown rGO nanosheets were dried in an oven overnight. Raman and FTIR techniques were used for rGO characterization.

2- Synthesis of and characterization $CeVO_4$ and SnS nanostructures

5mmol $Ce(NO_3)_3.6H_2O$ and 5mmol NH_4VO_3 were resolved in 40 mL of ultra-pure water (UPW) and mixed in a magnetic mixer for 30 min. 1M NaOH was supplemented until the pH of the solution was 10-12. 1.6 mmol $SnCl_2$·H2O, 80 µL thioglycolic acid (TGA) and 80 mM 160 mL Na_2S solution were mixed in a beaker for 10 min. Then each mixture were taken to separately Teflon-based hydrothermal containers and subjected to, 18 h for $CeVO_4$ and 15 h for SnS heat treatment at 180°C. The synthesized all nanostructures were separated via centrifuge and washed three times with UPW and 2 times with ethanol and dried overnight at 80°C. Synthesized all nanostructures were characterized via XRD and FESEM.

- Results



Equation	y = a + b*x
Plot	B
Weight	No Weighting
Intercept	0.20702 ± 0.0125
Slope	0.0033 ± 3.62715E-4
Residual Sum of Squares	0.00351
Pearson's r	0.96557
R-Square (COD)	0.93233
Adj. R-Square	0.92105

Fig 1. CV curve (A) and calibration curve (B) of prepared ITO/rGO@SnS@$CeVO_4$ composite electrode with different concentration of tyrosine in PBS.

The CV curves and the corresponding calibration curve of the tyrosine measurements made with the photosensitive ITO/rGO@SnS@$CeVO_4$ composite sensors in solutions containing different concentrations of tyrosine are shown in Fig. 1. As can be seen from the calibration curve, the fabricated sensor operates linearly in the concentration range of 1-75 µM. In addition, the LOD, LOQ, and sensitivity values were determined as 0.056 µM, 0.186 µM, 351 µA mM^{-1} cm^{-2}, respectively. The developed photosensitive ITO/rGO@SnS@$CeVO_4$ sensor was found to have good selectivity, low interference effect, reproducible and high long-time stability values.

- Discussion

A new photosensitive tyrosine sensor has been developed using ITO/rGO@SnS@$CeVO_4$ triple composite electrode materials. Thanks to the photosensitivity of rGO and the high electron permeability and stable structure of $CeVO_4$, electron transfer has been successfully achieved in the developed photosensitive tyrosine sensor.

- References

[1] Kamble, C., Chavan, R., Kamble V., A Review on Amino Acids, Research & Reviews: A Journal of Drug Design & Discovery, 2021; 8(3): 19–27p.
[2] Akram, M., Asif H.M., Uzair, M., Akhtar, N., Madni, A., Ali Shah, S.M., Hasan, Z., Ullah, A., Journal of Medicinal Plants Research, 2011; 5(17), 3997-4000.

O7. Electrochemical sensing of gallic acid based on GCE/TiO_2/ZnS nanocomposites

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Abstract

In this study, GCE/TiO_2/ZnS nanocomposite has been used to determined gallic acid (GA) in food samples. The electrochemical oxidation process of GA is investigated on a glassy carbon electrode (GCE). ZnS and TiO_2, which are selective and highly sensitive semiconductor materials, are used for detection of GA. The high sensitivity, high selectivity and reproducible gallic acid analysis was performed via GCE/TiO_2/ZnS composite electrochemical sensor in this study.

Introduction

Gallic acid is a member of polyphenols, also known as 3,4,5-trihydroxybenzoic acid. It has a chemical structure of $C_6H_2(OH)_3CO_2H$. Gallic acid has a crystal structure and a yellow-white color. It is easily soluble in water, it has the capacity to dissolve in alcohol, ether and glycerol, while it is insoluble in chloroform and benzene. Gallic acid is found in various fruits such as strawberries, grapes, bananas, blackberries, blueberries, avocados, currants, mangoes, mulberries, pomegranates, apples, as well as various plant products such as sumac, green tea, hazelnut, oak and chestnut trees, and some barks [1].

It has been reported that gallic acid (GA) has anti-inflammatory, antihistamine, anti-tumor activity, which is closely related to human life and health, and has a protective effect on free radical scavenging and cardiovascular diseases. GA is mostly obtained from food, and therefore, food safety, which affects human health, has been the focus of attention of scientists in recent years [2]. Various methods such as chromatography, chemiluminescence and electrochemistry have been used to date for the qualitative and quantitative detection of GA in foods. However, there are some disadvantages in the application of these methods. Sensors as an alternative method to overcome the disadvantages of these methods have been the focus of attention in recent years. There are many studies in the literature, especially on biochemical and chemical sensors, and these studies offer the opportunity to detect polyphenols at ppm level. In order to increase the efficiency of sensors, the use of nanostructures and their composites in sensors has become widespread in recent years [3].

Method

ZnS and TiO_2 Synthesis: 1.83g $Zn(NO_3)_2.6H_2O$ and 1.49g $Na_2S.9H_2O$ were resolved in 40 mL ultrapure water and mixed for 30 min. The mixture transferred to the Teflon lined hydrothermal reactor was heated at 180°C for 12 h. 5 mL of 1M NaOH solution was taken and mixed with 5 mL of titanium isopropoxide for 30 min. The mixture was transferred to a Teflon lined container and TiO2 nanoparticles were synthesized using microwave assisted hydrothermal procedure at 100°C and 380 W for 45 min. The formed ZnS and TiO2 nanoparticles were several washes with distilled water and methanol to remove impurities followed dried overnight in an oven at 80°C.

Electrochemical sensor preparation: 5 mg/L TiO_2 NP and 5 mg/L ZnS NP were dispersed in methanol, separately. GCE electrodes were cleaned with 0.5 µm alumina powder and in water methanol and acetone, respectively. Then, 4 µL of TiO_2 suspension was dropped on GCE electrode, and after drying, 4 µL of ZnS NP dropped onto GCE/TiO_2 electrode to prepare composite sensors.

Results

A new gallic acid sensor has been developed using ZnS and TiO_2 NPs as electrode materials. Thanks to the high surface area and catalytic activity of ZnS and TiO_2, electron transfer has been successfully achieved in the fabricated electrochemical GA sensor.

Whereas TiO_2 has high surface area, high conductivity and strong adsorption ability, ZnS is exhibited high catalytic activity and high conductivity. The electrochemical sensor studies of prepared GCE/TiO_2/ZnS were carried out by linear sweep voltammetry (LSV), cyclic voltammetry (CV), differentiated pulsed voltammetry (DPV) and electrochemical impedance spectroscopy (EIS) techniques.

Crystal structures of TiO_2 and ZnS were investigated by XRD characterization. It was observed that the examined TiO_2 structure was compatible with ZnS. Using electrochemical impedance spectroscopy, the resistances of the sensor formed with different electrodes were measured and compared with each other. Electrochemical sensors are known as more selective, reliable and sensitive devices compared to other devices, and they also have advantages such as faster response times, lower costs and ease of use. The reaction of GA as a reducing agent on the electrode surface is triggered by the applied potential and a current peak is produced by measuring the analyte concentrations generated.

Discussion

The composite electrode prepared using TiO_2 and ZnS reacted even at the lowest GA concentration and showed successful results in the electrochemically sensitive determination of GA. Last but not least, the developed photosensitive GCE/TiO_2/ZnS sensor promises to perform a sensitive and stable GA analysis.

References

[1] J. Zhao, I.A. Khan, F.R. Fronczek, Acta Crystallogr. Sect. E Struct. Reports. **67E**, o316-317 (2011).

[2] D. Bradley, Mater. Today. **13:6** 10-10 (2010).

[3] S. Yang, B. Yin, L. Xu, B. Gao, H. Sun, L. Du, Y. Tang, W. Jiang, F. Cao, Anal. Methods. **7** 4546–4551 (2015).

O8. Fabrication of Novel Gellan Gum or Polyvinylidene Fluoride Based Gels Containing LiTFSI, Self-Polymerized PEDOT and I^-/I_3^- Redox Couple

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Abstract

Gel electrolytes containing lithium bis(trifluoromethanesulfonyl)imide (LiTFSI), self-polymerized poly(3,4-ethylenedioxythiophene) (PEDOT) and I^-/I_3^- redox couple based on gellan gum (GG) or polyvinylidene fluoride (PVDF) were prepared in a one-pot reaction. Obtained gels were characterized via FTIR and contact angle. Both gels showed very low contact angle values. Furthermore, both gels have adhesive property.

Introduction

Renewable energy sources and energy storage systems have become important in the last years due to depletion of fossil fuels and environmental hazards they have caused [1]. Electrolytes are one of the crucial components of energy production and storage systems and provide charge transport between electrodes [2]. Traditional liquid electrolytes have been prepared with volatile solvents for dye-sensitized solar cells (DSSCs). The volatility of electrolytes creates problems such as leakage and instability of devices due to the loss of electrolytes. To overcome these problems, quasi-solid electrolytes, also known as gel electrolytes, have been investigated. These types of electrolytes eliminate leakage and electrolyte losses. In addition, gel electrolytes can show unique properties such as self-healing, anti-freezing or self-adhesiveness [3–5].

In this work, GG or PVDF-based gels containing LiTFSI, PEDOT and I^-/I_3^- redox couple were prepared in a one-pot reaction. While LiTFSI was used to increase ionic conductivity, PEDOT was included for enhancing covalent conductivity. Moreover, it was thought that prepared gel electrolytes could be used for flexible dye-sensitized solar cells.

Method

Redox couple solution was prepared by dissolving the appropriate amount with the final concentration of 0.05 M I_2, 0.5 M 4-tert-butyl pyridine and 0.1 M LiI in acetonitrile. GG or PVDF at a ratio of 5% w/v was added to preheated 25 mL DMSO to prepare gels. Solutions were mixed until GG or PVDF was fully dissolved. After that, the addition of the prepared redox couple solution was realized with a ratio of %25 v/v. Then LiTFSI and PEDOT were introduced into the solution at a ratio of 1.5% and 0.1%, respectively. Due to the insolubility of PEDOT in DMSO, 2 min ultrasonication was done to completely dispersion of PEDOT. Prepared gels were poured on Petri dishes while they were still hot and cooled to room temperature. Freeze-thaw cycles were applied twice to prepare gel electrolytes by bringing them to -20°C until entirely freezing and room temperature.

Results and Discussion

As can be seen in Figure 1a, desired gels based on GG or PVDF were synthesized successfully. In addition, it can be understood that LiTFSI and PEDOT were incorporated into the gels. Especially, the peak below 3000 cm^{-1} belongs to the sp^2 hybridized C-C bonds PEDOT contains.

Contact angle images can be seen in Figure 1b and Figure 1c. Both GG and PVDF gels showed very low contact angle values with an average of 5.2 and 0 for GG/LiTFSI/PEDOT and PVDF/LiTFSI/PEDOT, respectively. Additionally, it is known that there is an inversely proportional relationship between contact angle and surface energy, and adhesiveness increases with surface energy. Therefore, both gels showed self-adhesive property, as can be seen in Figure 1d and Figure 1e.

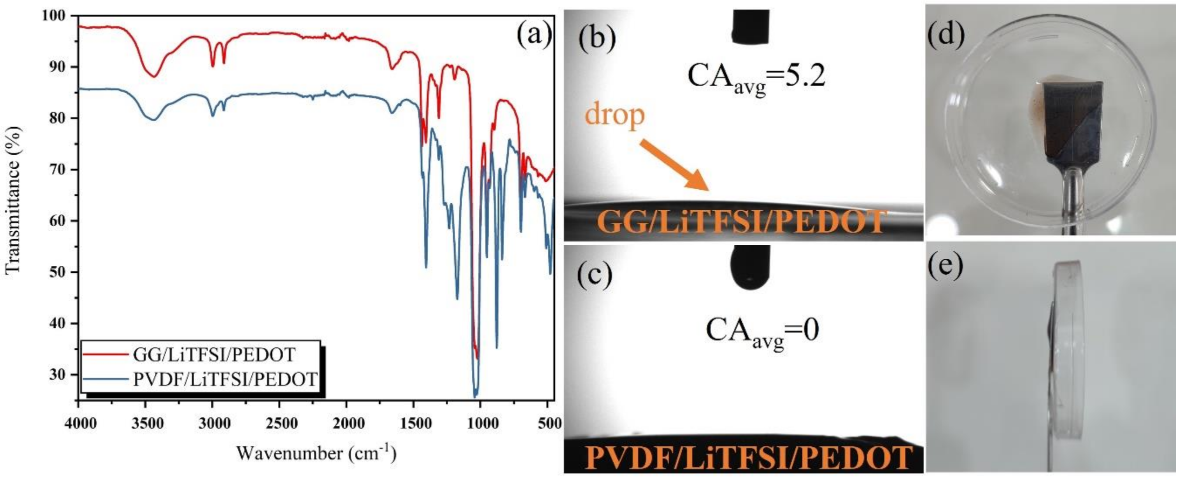

Figure 1. a) FTIR spectra of prepared gels, b,c) contact angle images of gels and d,e) images that show the self-adhesive property of gels

Conclusion

Both ionic and covalent conductive gels were synthesized successfully. Prepared gels showed very high hydrophilicity and self-adhesive property which makes them multifunctional material that can be used for different applications such as flexible dye sensitized solar cells.

Acknowledgement

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References

[1] H. Zhang, D. Yuan, J. Zhao, X. Ji, Y.-Z. Zhang, Gel Electrolytes: Chemistry and Applications, Chem. – An Asian J. n/a (2023) e202300360. https://doi.org/https://doi.org/10.1002/asia.202300360.

[2] Z. Liu, Q. Yu, N. Oli, J.F.F. Gomez, S. Qiu, H. Tian, Q. Qiu, W. Sun, K. Li, Z. Liu,

M. Chen, J. Yuan, X. Wu, L. Xia, A Non-Volatile, Thermo-Reversible, and Self-Protective Gel Electrolyte Providing Highly Precise and Reversible Thermal Protection for Lithium Batteries, Adv. Energy Mater. n/a (2023) 2300143. https://doi.org/https://doi.org/10.1002/aenm.202300143.

[3] K. Tajima, H. Hotta, Y. Yamada, M. Okada, K. Yoshimura, Electrochromic switchable mirror glass fabricated using adhesive electrolyte layer, Appl. Phys. Lett. 101 (2012) 251907. https://doi.org/10.1063/1.4772938.

[4] H. Liao, W. Zhong, T. Li, J. Han, X. Sun, X. Tong, Y. Zhang, A review of self-healing electrolyte and their applications in flexible/stretchable energy storage devices, Electrochim. Acta. 404 (2022) 139730. https://doi.org/https://doi.org/10.1016/j.electacta.2021.139730.

[5] W. Zhou, J. Chen, M. Chen, A. Wang, A. Huang, X. Xu, J. Xu, C.-P. Wong, An environmentally adaptive quasi-solid-state zinc-ion battery based on magnesium vanadate hydrate with commercial-level mass loading and anti-freezing gel electrolyte, J. Mater. Chem. A. 8 (2020) 8397–8409. https://doi.org/10.1039/D0TA01033B.

O9. Contact angle and surface energy behavior of poly (vinyl alcohol)/ poly (ethylene glycol)/carbon nanotube/doxorubicin hybrid hydrogels

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- Abstract

In this study, it was aimed to improve the hydrophobic properties of polyvinyl alcohol/polyethylene glycol (PVA/PEG) hydrogels containing carbon nanotube (CNT) at different weight ratios, and the effect of the synthesized hydrogels on the contact angle and surface energy was investigated. The hydrogel solution was prepared from 8 wt% PVA and 5 wt% PEG400. After adding 8 mL of 2 ppm doxorubicin (DOX-HCl) and 0.5 wt%, 1 wt% and 1.5 wt% CNTs to the autoclaved PVA/PEG solution, the samples prepared with different contents were sonicated. It was found that the average contact angle increased from 14.77° (PVA/PEG/DOX) to 73.73° (PVA/PEG/CNT/DOX) and the surface free energy decreased.

- Introduction

Hydrogels are hydrophilic three-dimensional network structures that closely resemble living tissues. They are frequently preferred in biomedical applications, especially for their widespread use as smart drug/cell carriers [1]. Hydrophilic drugs released from hydrophilic polymers often have undesirable release kinetics and durations. Hydrophobic polymers can be used as alternative drug carriers to overcome this problem [2]. The design, synthesis and characterization of hydrogel materials can improve the weak properties of the hydrogel [3]. The main aim of the present study is to improve the hydrophobic properties of hydrophilic hydrogels using CNT.

- Method

The hydrogel solution was prepared from 8% PVA and 5% PEG400 components by weight. The prepared solution was autoclaved at 121 °C for 15 minutes, and literature reports that autoclaving support the gelation of the hydrogel solution[4]. After adding 8 mL of 2 ppm DOX and 0.5 wt%, 1 wt% and 1.5 wt% CNTs to the autoclaved PVA/PEG solution, the samples prepared with different contents were sonicated. This solution, which did not form agglomerations thanks to the sonicator, was given the form of a hydrogel by the freeze-thaw technique. In the freeze-thaw technique, the hydrogels were frozen at -80 °C for 16 h and thawed at room temperature for 8 h; this cycle was repeated four times. Figure 1 shows schematic presentation of preparation process of the hydrogel.

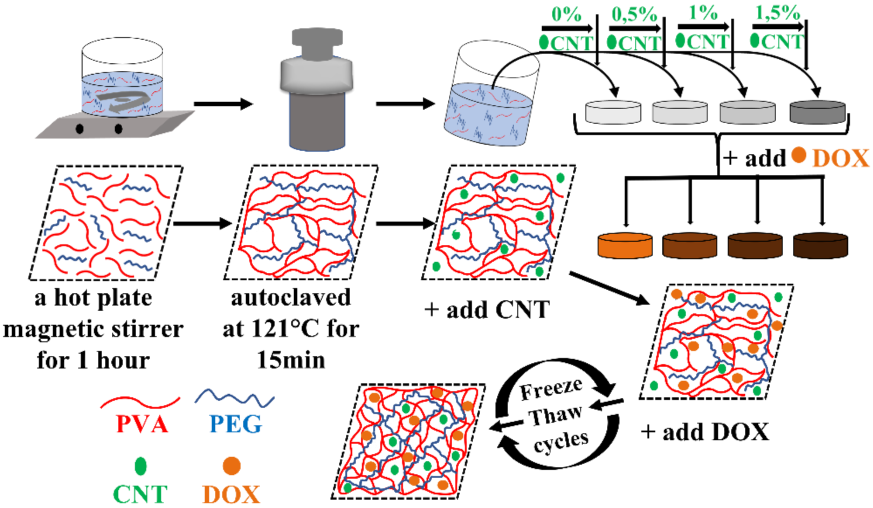

Figure 1. The schematic illustration of formation mechanism and preparation process of the hydrogel.

- Results

According to Figure 2 the mean contact angle was found to be 14.77° for hydrogel containing 0% CNT. The contact angle measurement of the 0.5% CNT hydrogel is 67.41° on average (Fig. 2 b). The average contact angle of the hydrogel containing 1% CNT is 69.75° (Fig. 2 c). Finally, the average contact angle of the hydrogel with 1.5% CNT is 73.73° (Fig. 2 d).

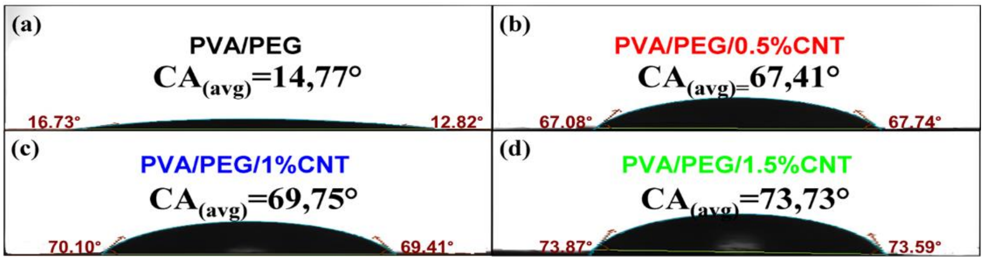

Figure 2. Hydrogels contact angle values measured with water.

Free surface energies were calculated automatically according to different methods with the help of a computer software program in the contact angle measuring device. According to Table 1, it was observed that the surface energies decrease by increasing the CNT ratio of the hydrogels due to van der Waals forces and hydrogen binding.

Table 1. The free surface energies of hydrogels calculated by different methods.

	Surface free energy(mN/m)				
Hydrogels	WU	OWRK/Fowkes	Equation of State	Acid-Base	Zisman
PVA/PEG/DOX	75,6938	70,9335	61,6992	56,2837	50,1000
PVA/PEG/DOX/0,5%CNT	56,9909	53,8383	46,9261	53,1731	50,0471
PVA/PEG/DOX/1%CNT	56,2075	53,1233	46,1790	52,4547	49,9822
PVA/PEG/DOX/1,5%CNT	54,8903	51,9414	44,9023	50,9331	49,8311

- Discussion

PVA/PEG hydrogel is hydrophilic due to the presence of hydroxyl groups. PVA/PEG molecules can bind to hydrophobic regions on the CNT surface by van der Waals forces and hydrogen bonding. As the proportion of nonpolar groups increased as the CNT ratio increased, the hydrophobic character increased, hence the surface wettability decreased and the contact angle increased and the surface energies of the hydrogels decreased as the contact angle increased [5].

References

[1] Avais M, Chattopadhyay S. Waterborne, *Polymer*, 180, 121701 (2019).
[2] Zhao X, Yildirimer L, Lin ZY, Cui W, *Nanobiomaterials in Drug Delivery*, 9, 403-445 (2016).
[3] Hughes GA, *Nanomedicine: Nanotechnology, Biology and Medicine*, 1, 22-30 (2005).
[4] Yamashita Y, Ohzuno Y, Saito Y, Fujiwara Y, Yoshida M, Takei T,Gels,9,280(2023).
[5] Gürbüz R, Sarac B, Soprunyuk V, Yüce E, Eckert J, Ozcan A, *Polym Adv Techno,* 32, 248–61 (2021).

O10. Ink Preparation for Supportless 3D Printing Of PVA/ALG/HA Composite Scaffolds

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Abstract

Additive manufacturing technologies are increasingly used for the fabrication of composite scaffolds. FDM is one of the widely used and cost-effective additive manufacturing techniques for the fabrication of patient-specific porous 3D scaffolds. In the study, a slurry and bath solution was prepared for 3D printing of antimicrobial polyvinyl alcohol (PVA), alginate (Alg) and Hydroxyapatite (HA) scaffold composites. Gluteraldehydride is used as the crosslinking agent in the preparation of the bath solution. In this study, HA/PVA and HA/PVA/Algae inks were successfully prepared for 3D printing in bath solution.

Introduction

With the recent development of additive manufacturing, a variety of polymers and ceramics are being used to fabricate scaffold structures that can induce bone regeneration. Biopolymer and bioceramics such as poly(vinyl alcohol)(PVA), poly(vinylpyrrolidone) (PVP), polylactic acid (PLA), polyglycolic acid (PGA), polycaprolactone (PCL), alginate, gelatin, silk, fibrin Hydroxyapatite(HA), calcium phosphate ceramics and bioglass are widely used in bone tissue engineering [1,2]. Extrusion based 3D printing is one of the additive manufacturing techniques in which involves the layer-by-layer deposition of materials through a nozzle or printing head. Rheological behaviour and shear thinning behaviour are important parameters which affect the printer ability of the ink [3]. The viscosity of the ink should be optimized so that it is easily extruded from the nozzle and quickly recovers its solid-like state after printing. Extrusion based 3D printing method have been modified and named as Coagulations bath, Direct ink printing (DIW), Freeform reversible embedding and Co-axial wet spinning [4,5]. Each extrusion-based manufacturing techniques has its own pro and cons. In coagulation bath technique, hydrogel materials is extruded in a bath solution that consist of crosslink agent to prompt immediate ionic crosslinking [5].

In this study PVA/HA/Alg composite ink and gluteraldehydrid(Ge) bath solution are prepared for scaffold printing. The printability of the PVA/HA/Alg composite will be determined by analyzing its rheological behaviour and the size change in shape in the bath solution.

Materials Method

Polyvinyl alcohol (MW = 89,000–98,000) and Hydroxyapatite (HA) powder were purchased from Sigma Aldrich, USA. Sodium alginate of 98% purity is used in ink preparation. PVA was mixed with the concentrations of 50% HA and 5% by total weight of alginate was added. 0, 5 and 10 v/v % glutaraldehyde was added to ethanol and deionized water to prepare bath solution. To prepare the mixture, PVA first dissolved in deionized water at 90 °C using magnetic stirrer. Then, alginate was dissolved in deionized water and added to the PVA mixture. Finally, HA powder was added to this mixture in different concentrations and mixed at 90 °C using magnetic stirrer until the desired viscosity was reached.

Rheological properties of ink samples were performed by a Rheometer (Anton Paar MCR 302, Austria). All rheology tests were performed by a Rheometer using a parallel plate setup at 24 °C, a shear stress of 1 Pa, and the angular frequency ω range from 0.1 to 100 rad/s. The ink's solidification will be determined by observing the droplet shape dropped into the bath solution containing the crosslinking agent after 30 s.

Results and Discussion

Print-friendly materials ideally provide consistent flow and reproducible fabrication [6]. In material extrusion 3D printing, ink is filled in a syringe and extruded through a nozzle and deposited layer by layer to build the desired object. The viscosity of ink may change when a force is applied to the syringe to flow ink through the nozzle. Shear thinning behaviour of the non-printed PVA/HA and PVA/HA/ (5%) ALG inks are shown in Figure 1. The decrease in viscosity of both inks with the increase in shear rate indicates that the ink becomes easier to flow or more liquid-like as the shear rate increases. Adding Alg to the HA/PVA mixture decreases the viscosity of the ink with an increase in shear rate [7].

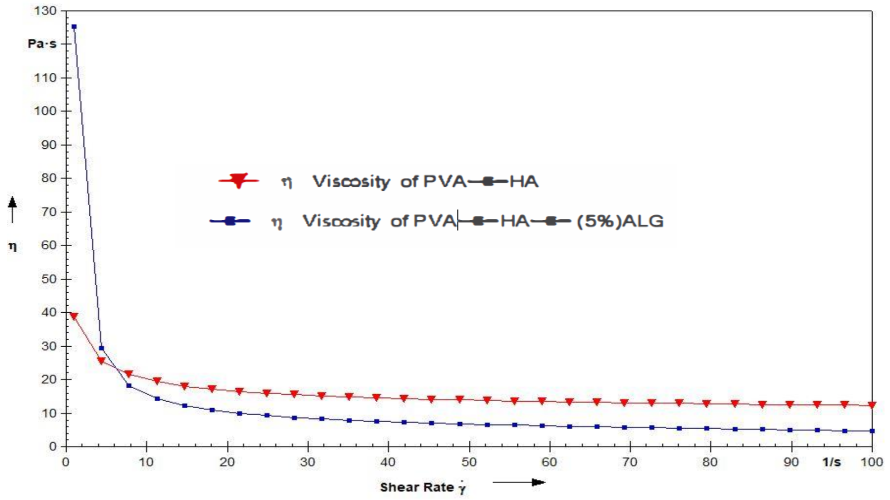

Figure 3. Shear thinning behaviour of the non-printed PVA/HA and PVA/HA/ (5%) ALG inks.

Shape of the ink droplets at 5 seconds and 60 seconds after being dropped into the bath solution. When the inks are dropped into the water/ethanol mixture, the inks start to spread and dissolve. Most of the material dissolves after 60 s. The inks being dropped in Ge bath solution continues to hold its shape and solidify. The solidification of the ink after 5 s and 60 s means that during 3D printing it will solidify until the next layer.

Conclusion

In this study, HA/PVA and HA/PVA/Algae inks were successfully prepared for 3D printing in the bath solution. The viscosity and rheological behavior of the material are important factors affecting the material's ability to 3D printing. The material must have a viscosity that can be extruded through the nozzle and not spread after extruding. This lower viscosity can be advantageous in 3D printing as it allows for smoother extrusion and more precise deposition of the ink, leading to improved print quality and accuracy. Extruding the material in a crosslink agent bath solution ensures rapid solidification of the material.

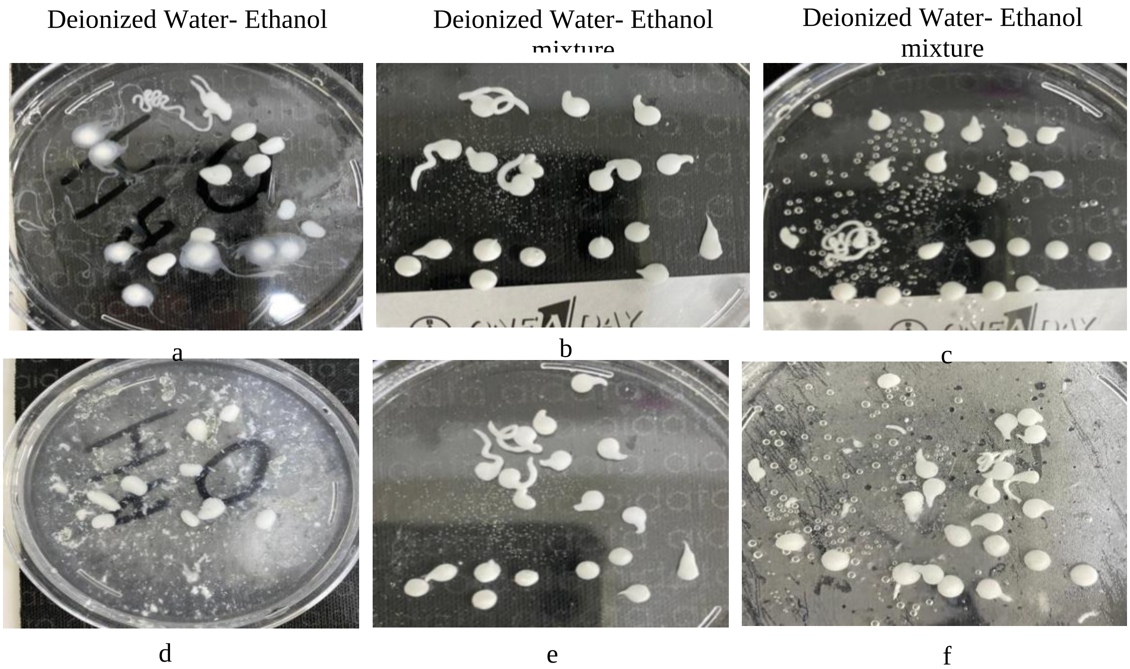

Figure 4. Shape of the ink droplets at 5 seconds and 60 seconds after being dropped into the bath solution. a), b) and c) after 5 seconds. d), e) and f) after 60 seconds.

Acknowledge:

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References

[1] N.M. Ergul, S. Unal, I. Kartal, C. Kalkandelen, N. Ekren, O. Kilic, L. Chi-Chang, O. Gunduz, 3D printing of chitosan/poly(vinyl alcohol) hydrogel containing synthesized hydroxyapatite scaffolds for hard-tissue engineering, Polym. Test. 79 (2019) 106006. https://doi.org/10.1016/j.polymertesting.2019.106006.

[2] M. Teodorescu, M. Bercea, S. Morariu, Biomaterials of PVA and PVP in medical and pharmaceutical applications: Perspectives and challenges, Biotechnol. Adv. 37 (2019) 109–131. https://doi.org/10.1016/j.biotechadv.2018.11.008.

[3] B.N. Turner, R. Strong, S.A. Gold, A review of melt extrusion additive manufacturing processes: I. Process design and modeling, Rapid Prototyp. J. 20 (2014) 192–204. https://doi.org/10.1108/RPJ-01-2013-0012.

[4] M. Costantini, C. Colosi, W. Święszkowski, A. Barbetta, Co-axial wet-spinning in 3D bioprinting: State of the art and future perspective of microfluidic integration, Biofabrication. 11 (2019). https://doi.org/10.1088/1758-5090/aae605.

[5] Y. Zheng, Y. Wang, F. Zhang, S. Zhang, K.D. Piatkevich, N. Zhou, J.K. Pokorski, Coagulation Bath-Assisted 3D Printing of PEDOT:PSS with High Resolution and Strong Substrate Adhesion for Bioelectronic Devices, Adv. Mater. Technol. 7 (2022) 2101514. https://doi.org/10.1002/admt.202101514.

[6] F. Fayyazbakhsh, M.J. Khayat, M.C. Leu, 3D-Printed Gelatin-Alginate Hydrogel Dressings for Burn Wound Healing: A Comprehensive Study, Int. J. Bioprinting. 8 (2022) 274–291. https://doi.org/10.18063/ijb.v8i4.618.

[7] S.T. Bendtsen, S.P. Quinnell, M. Wei, Development of a novel alginate-polyvinyl alcohol-hydroxyapatite hydrogel for 3D bioprinting bone tissue engineered scaffolds, J. Biomed. Mater. Res. Part A. 105 (2017) 1457–1468. https://doi.org/10.1002/jbm.a.36036.

O11. Anti-genic Effect of Green Synthesized Zinc Oxide Nanoparticles on Biofilm Gene Expression in MDR uropathogenic *E.coli*

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Biofilm forming bacteria possess a serious threat to human and animal health. This study aimed to investigate the effect of green zinc oxide nanoparticles (ZnO-NP) on biofilm formation and expression of the *MotA, MqsR, FliA, LuxS* and *FimH* genes in uropathogenic *Escherichia coli* (UPEC) strains.The green ZnO-NPs was synthesized by biological method using leave extract of Pomegranate (Punica granatum) plant. The antibacterial and anti-biofilm effect of synthesized green ZnO-NPs were evaluated by agar well diffusion and macrotiter dilution method to determine (MIC, SUB-MIC values with control). Anti-gene expression of biofilm encoding genes of *E.coli* (MotA, MqsR, FliA, LuxS and FimH) were evaluated by Real- time quantitive polymerase chain reaction (RT-qPCR) before and after treatment with Zinc oxide nanoparticles.

The results showed that the most common bacterial isolates were *E.coli* (30 in UTI Human, 20 in UTI Animals), and the diagnosis was confirmed by Vitek system. Forty six (92%) biofilm producer isolates from (human and animal) after phenotypically biofilm detection assay with congo red and tissue culture plate methods and genetically using (RT-qPCR). Also, the green ZnO-NPs have a significant inhibitory effect on biofilm bacteria. The activity green zinc oxide nanoparticles were effective on biofilm gene expression by down regulate expression of these genes. Green ZnO-NPs showed an excellent inhibitory effect and anti-biofilm activity against MDR biofilm E. coli and It may be a promising solution in the future to eliminate bacteria that are resistant to antibiotics as alternative means to antibiotics.

O12. Corrosion assessment of nickel electrowinning coatings from watts bath in 0.5N NaCl

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Electrodeposited nickel coatings are used in industry to improve surfaces appearance, better corrosion protection, hardness, wear, magnetic and other properties. This work aims to characterize electrodeposited Nickel coatings on copper substrate from watts bath at different temperatures by evaluating their corrosion resistance in 0.5N NaCl solution. The microhardness, the electrochemical behavior and the corrosion properties of the deposited layers were evaluated by d.c polarization such as cyclic voltammetry, open circuit potential (OCP), potentiodynamic techniques, electrochemical impedance spectroscopy EIS and Vickers microhardness. While the surface morphology was evaluated by optic microscopy and white light interferometer (WLI). It was found that increasing the bath temperature to 55°C leads to a smoother, dense, compact and recovering Ni coatings with a decrease in the grain size and average roughness. In addition, it was shown that the coatings elaborated at 55°C have the highest corrosion resistance in 0.5N NaCl solution with charge transfer resistance "Rct" value of 58387 Ω/cm². Investigation of the mechanical properties of the coating elaborated at 55°C achieved the highest hardness value of 113.4 Vickers.

O13. Local piezoelectric properties of Di-Leucine dipeptides nanotubes

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Di-peptides nanotubes (PNTs) have received much attention in the last decade because of their close relationship with life and the nanotube formation by various hydrophobic dipeptides and its structural properties [1, 2]. These are materials absolutely corelated with biology (systhesis, physical and chemical properties, utilizations) and their have many potential applications in various broadening fields from medicine (as containers for medical, biosensors, etc. to technology energy (harvesting), nanoelectronics, Semiconducting Nanostructures, colored surfaces. PNTs are as well as genetic and tissue (protein) engineering. Tubular structures can be constructed with cyclic di-, tri-, tetra-, hexa-, octa-, and decapeptides with various amino acid sequences, enantiomers, and functionalized side chains

Di-Leucine (LL) peptide nanotubes (PNTs) were grown. The local piezoelectric properties of LL PNTs were measured using atomic force microscopy. Using piezoresponse force microscopy (PFM) the strong piezoelectric properties with d_{15} = ~3.2 pm/V was found. The magnitude and distribution of the piezo response signal were analysed depending on the orientation of the tubes. Features of the charge distribution depending on the microstructure of LL PNTs were discovered by Kelvin Probe Force Microscopy.

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

References

[1] C. H. Gorbitz, Nanotube Formation by Hydrophobic Dipeptides, Chem Eur J., 7, 5153–5159 (2001).
[2] E. Gazit, A possible role for π-stacking in the self-assembly of amyloid fibrils, FASEB J., 16, 77-83 (2002).

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O14. Synthesis of Fe_3O_4 magnetic nanoparticles, modifying with tannic acid and loading and releasing application of salicylic acid

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Abstract

In this study, Fe_3O_4 magnetic nanoparticles (MNPs) were synthesized using a co-precipitation method, followed by the binding of tannic acid onto the nanoparticle surface. The prepared MNPs were then utilized for the loading and releasing application of salicylic acid, a widely used therapeutic agent. The synthesis process was characterized using various analytical techniques, and the loading and releasing behavior of salicylic acid from the nanoparticles were evaluated. The results demonstrated the successful synthesis of Fe_3O_4 MNPs and the effective binding of tannic acid. The loading and releasing of salicylic acid exhibited controlled and sustained release profiles, indicating the potential of these MNPs as drug carriers.

Introduction

Fe_3O_4 MNPs have gained significant attention in the field of drug delivery due to their unique magnetic properties and biocompatibility. The binding of organic molecules onto the nanoparticle surface allows for functionalization and controlled release of therapeutic agents. Tannic acid, a polyphenolic compound, possesses excellent binding capabilities and has been utilized for surface modification of MNPs. Salicylic acid, known for its anti-inflammatory and antimicrobial properties, is served as a model drug in this study for loading onto the MNPs. [1]. The study provides insights into the synthesis of Fe_3O_4 MNPs, their functionalization with tannic acid, and their application in loading and releasing salicylic acid, highlighting their potential for controlled drug delivery systems.

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. The mixture was heated to 80 °C and stirred at 150 rpm for 1 h. Subsequently, 22.5 mL of ammonia solution was rapidly added to the mixture and stirred for another hour under nitrogen atmosphere. The resulting MNPs were then cooled to 25 °C. Afterward, the MNPs were washed three times with distilled water and once with ethanol. Finally, they were dried at 65 °C for 24 hours 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 [2].

Results

The synthesized Fe_3O_4 MNPs exhibited a crystalline structure and uniform size distribution, as confirmed by XRD and SEM analysis. The successful binding of tannic acid onto the nanoparticle surface was confirmed by FTIR spectra. The loading of salicylic acid onto the MNPs was achieved, and the release behavior was characterized by sustained and controlled release profiles [3].

Discussion

The synthesis of Fe_3O_4 MNPs via the co-precipitation method provided nanoparticles with desired properties for drug delivery applications. The binding of tannic acid onto the nanoparticle surface improved the stability and dispersibility of the nanoparticles. The loading and releasing of salicylic acid demonstrated sustained release behavior, indicating the potential of these MNPs for controlled drug delivery systems.

References

[1] S. Ananthi, M. Kavitha, E.R. Kumar, A. Balamurugan, Y. Al-Douri, H.K. Alzahrani, A.A. Keshk, T.M. Habeebullah, S.H. Abdel-Hafez, N.M. El-Metwaly, Sensors and Actuators: B. Chemical, 390, 131071 (2021).
[2] H. Veisi, S.B. Moradi, A. Saljooqi, P. Safarimehr, Mater. Sci. Eng. C, 100, 445-452 (2019).
[3] H. Veisi, M. Pirhayati, A. Kakanejadifard, P. Mohammadi, M.R. Abdi, J. Gholami, S. Hemmati, ChemistrySelect, 3, 1820-1826 (2018).

O15. Electrochemical performance of Cu_2O anode material synthesized by electrodeposition method for rechargeable lithium-ion batteries

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Cu_2O is currently used for numerous applications, including gas sensors, solar energy conversion, photocatalysis and batteries. Recently, Cu_2O has received more attention for the anode application of the rechargeable Lithium-Ion Battery (LIB) than the other competing materials because of its high theoretical capacity (375mAhg^{-1}), good capacity retention, affordability, non-toxicity and ease of storage. The electrochemical performance of Cu_2O mainly depends on its crystallinity and morphology that significantly depend on the synthesizing technique. The electrodeposition method, which is a promising technique that improves the crystallinity with favorable morphology for electrode materials, has not been studied well for synthesizing Cu_2O. Hence, this study aims for preparing Cu_2O anode materials by the electrodeposition method with enhanced crystallinity and morphology. The coin cells were assembled in an argon-filled glove box with anodes fabricated with synthesized Cu_2O, lithium as the reference electrode and counter electrodes together with the non-aqueous electrolyte of 1M $LiPF_6$ in ethylene carbonate and dimethyl carbonate (1:1wt%). The galvanostatic charge-discharge tastings performed on the assembled coin cells showed a significantly high initial specific discharge capacity of 533 mAhg^{-1} while maintaining high Coulombic efficiency of around 99% over 50 cycles. Even though it reported a higher irreversible capacity of 362.3 mAhg^{-1} at the 1st cycle, it showed a significantly lower irreversible capacity of 0.2 mAhg^{-1} for the 50th cycle. Electrochemical impedance spectroscopy and cyclic voltammetry analyses also provide improved electrochemical performance. Altogether this study reveals that Cu_2O synthesized by electrodeposition method processes very promising electrochemical performance for the anode application of LIB.

O16. Developing Vein Graphite Anode Materials for Li-ion Batteries by Optimizing and Scaling up of Chemically Mild Oxidation

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Vein graphite has emerged as a potential intercalating anode material for rechargeable Li-Ion Batteries (LIBs). However, the formation of Solid Electrolyte Interface causing a large irreversible capacity loss during the first lithium intercalation is still a challenging obstacle. To address this obstacle, it is crucial to eliminate structural imperfections in graphite that hinder the electrolyte decomposition, block intercalation of solvated Li-ions, and prevent graphene planes from migrating along the a-axis direction. Therefore, surface modification methods have been introduced by primarily focusing on mild oxidation, alkali carbonate coating and Li-doping methods. Among the various surface modification approaches for vein graphite, chemically mild oxidation using HNO3 acid method (NO method) was selected as the most promising technique after a thorough optimization of critical factors and parameters. Prior to scaling up, the NO method was further optimized to enhance surface modification and ensure the purity of graphite. Following successful optimization, this study was extended to investigate the feasibility of scaling-up at the laboratory level, as possible. The outcome of the optimization process revealed that the volume of 50 ml of 69.0% HNO3 acid as the optimum condition for the scaling-up. The scaled-up vein graphite samples obtained using the NO method showed similar characteristics to the initial laboratory sample, with a purity level of 99.0%, rendering their suitability for LIB anodes. Moreover, the electrochemical performance of the scaled-up graphite samples is promising by behaving in a manner consistent with the initial laboratory sample, despite a low discharge capacity initially. These findings confirm the effective scaling-up of the NO method at the laboratory level. The successful laboratory scale implementation of this method represents a significant improvement and lays the foundation for a scale-up framework for future development. Thus, this study paves the way for future research and development to establish a comprehensive laboratory level scale-up approach that endeavors towards the ultimate usage of vein graphite in LIB anode.

O17. Artificial Knee Implant Design and Analysis with Finite Element Method

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- Abstract

The human body is a perfect machine in which different systems and structures coexist. A large number of bones that make up the skeletal structure of the body and carry all the weight move in harmony with the help of joints [1,2]. The knee joint is one of the most complex of these structures [3]. The knee joint loses its functions due to old age, accident, injury, etc. In the knee joint, there is a cartilage structure that is in contact with each other during movement and allows the movement to take place painlessly. In the article, the deformation and stress values of the cartilage structure by applying different pressure forces on the artificially designed knee joint were examined by the Finite Element method. The knee joint, which was designed from four different materials, was analyzed in 5 different wall thicknesses and the most appropriate knee implant model was tried to be determined by interpreting the results obtained.

- Introduction

The largest and most complex joint in the human body is the knee joint [2,3]. The knee joint has the widest and most complex synovial membrane anatomically [3]. A lubricating fluid is naturally present in the joints [4]. The slippery and colorless fluid is called synovial fluid. The synovial membrane responds to damage to the knee joint by producing fluid. Over time, fluid loss occurs in the knee joint due to osteoarthritis, aging, disproportionate use of the knee joint, etc [5]. After diagnosing fluid loss in the knee, treatment methods are determined [6,7]. These methods can be listed as drug treatments, diet and weight loss applications and artificial liquid injections. Another way to solve this problem is to implant a new cartilage structure by surgical operation [8]. The aim of knee cartilage transplantation is to improve the patient's quality of life and mobility [9].

The aim of this study is to analyze the cartilage structures designed in different materials and sizes, which will help the treatment, with the finite element method and to compare them in terms of strength. As a result, the type of material, pressure force, cost, strength and displacement parameters that we think affect the knee joint design are examined theoretically and the results are interpreted.

- Method

In the study, SolidWorks software was used for computer aided design (CAD) and modeling, and ANSYS WorkBench software was used for finite element analysis. The CAD model and network structure designed and used in the analysis are shown in Figure 1.

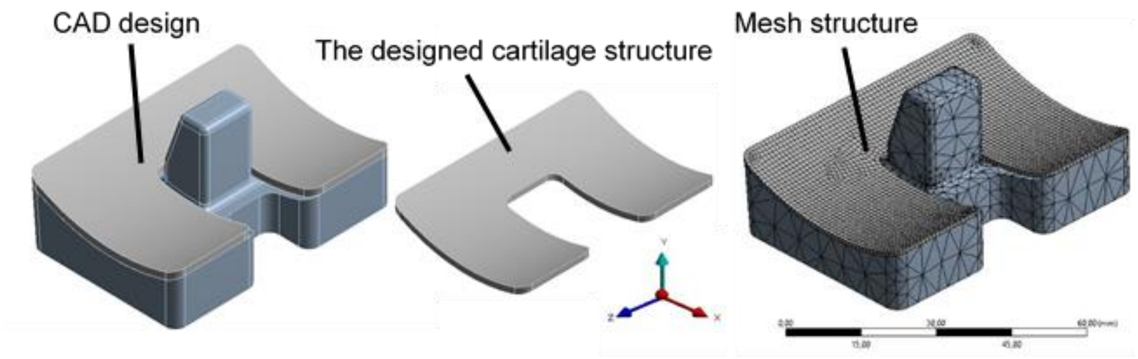
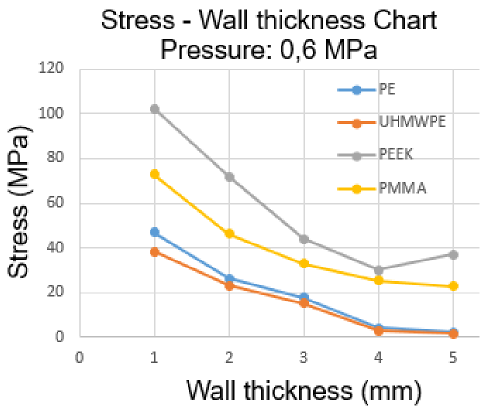


Figure 1. Knee implant CAD design and Mesh structure.

During the analyses, a compressive force was applied on the cartilage structure modeled in different wall thicknesses and the resulting stress and deformations were examined.

- Results

Depending on the wall thickness, the stress decreases, while the deformation increases. It was determined that the highest deformation was in UHMWPE material and the lowest deformation was in PEEK material. As the pressure force increases, the deformation increases at the same rate. Figure 2 and Figure 3 show the stress and deformation values that occur when a pressure of 0.6 MPa is applied.



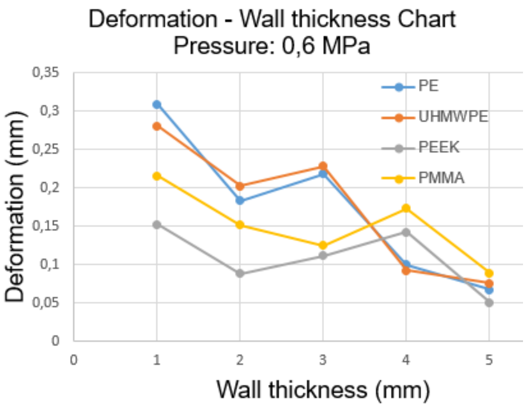


Figure 2. Stress-Wall thickness chart **Figure 3.** Deformation-Wall thickness chart

- Discussion

The lowest stress occurs in the UHMWPE material and the decrease in the stress value increases as the wall thickness increases. Although a similar change is observed in PE material, the stress values are higher. When the deformation values are examined, the highest deformation occurs in the UHMWPE material. The lowest deformation is in PEEK material. The wall thickness significantly affects the stability of the cartilage structure. If the wall thickness is 3 mm, the most suitable results were obtained in terms of stress, deformation and strain. It would be beneficial for the cartilage structure to have a wall thickness of 3mm or higher in order to function for a longer period of time. However, there must be sufficient space in the area where the cartilage structure will be placed.

References

[1] L.F. Samhan, A.H. Alfarra, S.S. Abu-Naser, *International Journal of Academic Information Systems Research*, 2021, **5**, 59.

[2] J. Prathap Kumar, M. Arun Kumar, D. Venkatesh, *International Journal of Current Research and Review*, 2020, **12**, 1.

[3] J.F. Abulhasan, M.J. Grey, *Journal of Functional Morphology and Kinesiology*, 2017, **2**.

[4] D. Ne *et al.*, *Biotribology*, 2019, **17**, 1.

[5] M.H.M. Yunus, A. Nordin, H. Kamal, *Medicina (Lithuania)*, 2020, **56**, 1.

[6] H. Li *et al.*, *Molecular Medicine Reports*, 2016, **13**, 2071.

[7] A. Kendall, S. Ekman, E. Skiöldebrand, *Journal of Orthopaedic Research*, 2023, **41**, 316.

[8] S. Bhandarkar, P. Dhatrak, *Materials Today: Proceedings*, 2022, **59**, 459.

[9] H.D. Clarke, K.R. Math, G.R. Scuderi, *The Journal of Arthroplasty*, 2004, **19**, 652.

O18. Surface characterization of CNT coated aluminum alloy

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Abstract

Aluminum alloys are widely used in the aerospace and automotive fields. Due to the needs in increasing application areas, there is a need for detailed examination of Al coatings. In this study, CNT coated Al substrates (Coated Al-1, Coated Al-2 and Coated Al-3) were obtained. FTIR and contact angle characterizations were carried out after drying the Al substrates with different densities of coatings by the drop-casting method for 24 hours. Contact angles were determined as 123.8°, 99.8°, 92.7° and 92.0° for Pristine Al, Coated Al-1, Coated Al-2 and Coated Al-3 samples, respectively.

1. Introduction

Aluminum alloys are the materials with wide application on the automotive and aerospace area. Surface coating and functionalization of alloys are important for their properties such as increasing their mechanical strength and increasing corrosion resistance [1,2].

Carbon nanotube (CNT), which is among the nanomaterials, has been studied for a long time. As a result of their mechanical strength and functionalization, they have found a place for themselves in a wide area [3,4].

Due to the increasing needs in the field of high-strength and multi-functional spacecraft and aircraft, coating materials made of aluminum alloy (Al) are in a remarkable position. Different compositions as coating materials have been used in the literature for purposes such as increasing mechanical strength, providing adhesive bonding, reducing corrosion. There is still a need for detailed examination and examination of the properties of multifunctional Al coatings with increasing material diversity.

In this study, CNT was successfully used on Al 2024-T3 substrate, coatings were carried out and surface characterizations were carried out.

2. Method

Firstly; CNT was suspended (2mg/mL) in concentrated acid. After mixing for 12 h and drying at 100°C for 3 h, oxidized CNT was obtained. Al substrates (25mmx25mm), which were previously cleaned with acetone in a sonic bath, were coated with CNT solutions obtained by drop-casting method. In order to obtain coated Al-1, Al-2 and Al-3 samples with different coating density, oxidized CNT solutions were dropped on the Al substrates in the ratios of 0.1, 0.2 and 0.4 mL/cm^2, respectively, and left to dry at room temperature overnight.

3. Results

The FTIR and contact angles of the Pristine Al sample, which is a comparison sample with Coated Al-1, Coated Al-2 and Coated Al-3 samples, were characterized. Considering the FTIR analyzes of the coated and uncoated samples (Fig. 1.A), the coating was confirmed by newly observed peaks. As shown in Fig1b with the images of the coating samples, the average contact angles for Pristine, Al-1, Al-2 and Al-3 samples were analyzed as 123.8°, 99.8°, 92.7° and 92.0°, respectively.

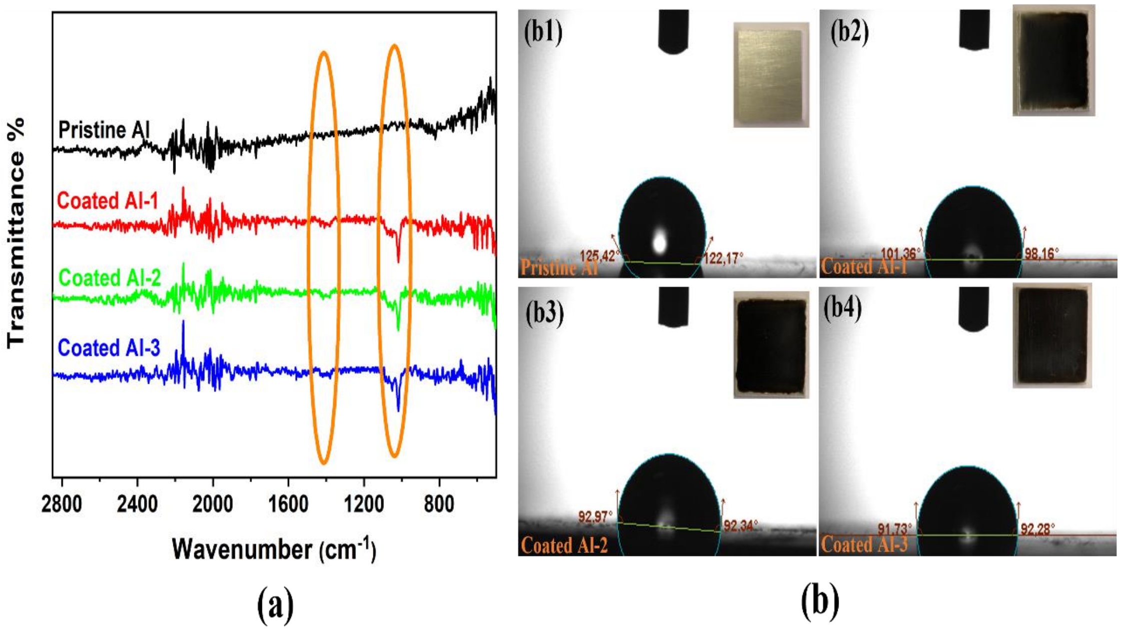

Figure 1. Images of (a) FTIR analysis and (b) contact angles of Pristine Al, Coated Al-1, Coated Al-2, and Coated Al-3 samples (coated samples inserted).

4. Discussion

Successful coating of CNT obtained after acid treatment on Al alloy substrate was observed by FTIR analysis. Considering the contact angles, it was observed that the decrease in the contact angle tended to decrease with the increase in the coating density. Compared to Pristine Al alloy, the decrease in the contact angle is caused by polar groups, while the decrease in the contact angle is thought to be due to the saturated interactions between the Al alloy substrate and the polar groups.

References

[1] M. Sattari, A. Olad, F. Maryami, I. Ahadzadeh, K. Nofouzi, Surfaces and Interfaces, **38**, 102860, (2023).
[2] P. Mayer, A. Dmitruk, J.W. Kaczmar, Int. J. Adhes. Adhes., **109**, 102899, (2021).
[3] A. Ali, S.S. Rahimian Koloor, A.H. Alshehri, A. Arockiarajan, J. Mater. Res. Technol., **24**, 6495–6521, (2023).
[4] P. Baghel, A.K. Sakhiya, P. Kaushal, Heliyon., **8,** 10943, (2022).

O19. Understanding the effect of fluoroethylene carbonate addition into an electrolyte - a molecular dynamics study

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Fluoroethylene carbonate (FEC) is used as an electrolyte additive of Li-ion rechargeable batteries to mitigate volume expansion of the anode during battery cycling. However, the effect of FEC addition on the electrolyte has not been studied adequately. Here we report molecular dynamics simulations of electrolyte mixtures commonly used in Li-ion batteries while focusing on the effect that varying FEC concentration has on the transport and solvation properties of other electrolyte components. Here, bonded and non-bonded force field parameters for the ethylene carbonate (EC), dimethyl carbonate (DMC) and FEC molecules were assigned using the Generalized Amber Force Field (GAFF) through Moltemplate. All the simulations were conducted using Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code. The systems were allowed to evolve for 2 ns first from their initial configuration. Once it was done, the simulations were further run for 30 ns. After this, 5 ns production runs were performed to collect the positions of atoms. The results showed that FEC addition, even as a minor component, has significantly affected the diffusion constants of species and total ionic conductivity of the electrolyte compared to those without addition. Moreover, the lithium ions show a lower rate of diffusion compared to hexafluorophosphate ions irrespective of FEC addition. Upon the addition of 10 % FEC, both lithium ions and hexafluorophosphate ions show a small increase in rate of diffusion. However, further addition has again decreased the diffusion of lithium ions. Further, Solvent species of ethylene carbonate and fluoroethylene carbonate show higher diffusion rate compared to lithium ions and hexafluorophosphate ions. Finally, these findings reveal that addition of FEC has changed the transportation and clustering properties of the EC/DMC/lithium hexafluorophosphate system.

O20. Synthesis, Water Retention Capacity and Swelling Behavior of Polyvinyl Alcohol/Carboxymethyl Cellulose Hydrogels Mimicking Dermis and Epidermis

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Abstract

In current study, hybrid hydrogels containing polyvinyl alcohol (PVA) and carboxymethyl cellulose (CMC) were investigated. PVA/CMC (4:4, 4:3, 4:2) was prepared in different ratios and the influence of CMC additive on the swell behavior and water retention capacity of the hydrogel was measured. As a result, it was observed that the hydrogel with a high amount of CMC showed similar properties to the epidermis.

Introduction

The skin is our largest organ and basically consists of three layers. These are epidermis, dermis, and hypodermis. Skin is subject to injuries throughout human life. Wound resulting from various work and home accidents, surgeries and burns are grouped under two headings: chronic wounds and acute wounds. In acute wounds, wound closure occurs within an acceptable time. In chronic wounds, this period is longer [1]. The main factor of wound healing is cell proliferation. Nowadays, it has been the subject of study of wound dressings and artificial skins to support cell proliferation. Wound dressings consist of many kinds such as alginate, hydrocolloid, hydrogel, polyurethane foam and nanofiber dressings. Artificial skin imitate the anatomical structure of the skin and can be produced by various methods. In this study, we introduce polyvinyl alcohol/carboxymethyl cellulose hydrogel artificial skin prepared to be both a wound dressing and a substitute for artificial skin.

Hydrogels are polymeric network structures with high water absorption capacity developed by various crosslinking methods. In physically crosslinked hydrogels, environmental factors can disrupt polymeric networks [2]. Therefore, chemical crosslinking agents are preferred during hydrogel production. Polyvinyl alcohol (PVA) is a biocompatible hydrophilic polymer [3]. PVA enables hydrogel production by both physical crosslinking and chemical crosslinking. Carboxymethyl cellulose (CMC) is a water-soluble derivative of cellulose [4]. Cellulose attracts attention because it is abundant in nature. CMC has been preferred in biomedical applications for reasons such as biocompatibility, biodegradability, transparency and low cost [5]. Citric acid (CA) is derived from citrus fruits, non-toxic and easily dissolved. Due to its non-toxicity, it has been preferred as a chemical crosslinker for hydrogel preparation in recent years [2].

Method

Hydrogel Production for Lower Layer. 1 g of PVA was resolved in 10 mL of distilled water (DW) magnetically stirring until a clear solution was obtained. Likewise, 0.5 g of CMC was resolved in 30 mL DW. The CMC solution was supplemented slowly to the PVA solution and mixing was continued. CA, a biocompatible crosslinking agent, was added to the PVA/CMC (2:1) solution at 20% by weight of the total polymer. The prepared solution was transferred into a petri dish and left at room conditions for 1 night to remove air bubbles. In order to provide physical crosslinking of the prepared hydrogel, freeze-thaw method was applied in 2 cycles.

Hydrogel Production for Upper Layer. The production steps for the lower layer are also valid for the upper layer hydrogel. Here, the CMC ratio and correspondingly the CA ratio have been increased in order to form tighter pores. Solutions were prepared in different containers as PVA/CMC (1:1 and 4:3). After the CMC solution was added to the PVA solution, CA was added at 20% by weight of the total polymer. The solutions were poured into petri dishes and after 1 night at room conditions, 2 cycles of freeze-thaw method was applied.

Results

Hydrogels were lyophilized for swelling analysis. Lyophilized hydrogels were placed in 15 mL falcon tubes and the tubes were filled with 10 mL distilled water. Swelling analysis continued until the water capacity of the hydrogels reached equilibrium (~90 min). S1 (PVA/CMC 2:1) and S2 (PVA/CMC 4:3) absorbed 5.7 and 6.25 times their dry weight, respectively, in the first 15 minutes (Figure 1). S3 (PVA/CMC 1:1), which is thought to have tighter and smaller pores with the increase in CMC and cross-linking, was able to absorb water only 3.1 times its dry weight in the first 15 min. Based on this, it can be said that S3 is suitable for the epidermis layer.

After 24 h of water absorption and expansion at room temperature, the mass of the wet sample was weighed to determine the water retention capacity of the hydrogels. Measurements were taken 4 times from the hydrogels placed in an oven at 37 °C. The water retention capacity of all the prepared hydrogels showed similar properties.

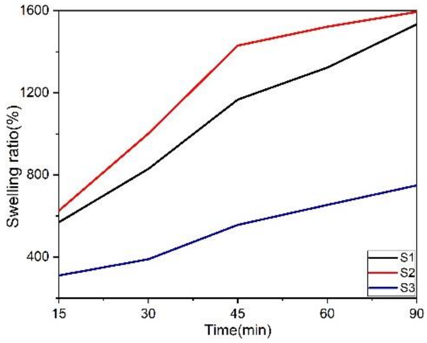

Figure 1. The swelling behavior of hydrogels as a function of time.

Discussion

The water retention capacities and swelling behaviors of hydrogels, which are produced in two stages and mimic the epidermis and dermis layers, were investigated. The hydrogels exhibited high swelling behavior and showed similar water retention capacity.

Acknowledgements

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References

[1] J. A. D. Whitney, Nursing Clinics of North America **40**, 191 (2005).
[2] K. K. Mali, S. C. Dhawale, R. J. Dias, N. S. Dhane, and V. S. Ghorpade, Indian J Pharm Sci **80**, 657 (2018).
[3] H. Adelnia, R. Ensandoost, S. Shebbrin Moonshi, J. N. Gavgani, E. I. Vasafi, and H. T. Ta, Eur Polym J **164**, 110974 (2022).
[4] V. S. Ghorpade, A. V. Yadav, R. J. Dias, K. K. Mali, S. S. Pargaonkar, P. V. Shinde, and N. S. Dhane, Int J Biol Macromol **118**, 783 (2018).
[5] Y. Li, C. Zhu, D. Fan, R. Fu, P. Ma, Z. Duan, X. Li, H. Lei, L. Y. Chi Li, C. Zhu, D. Fan, R. Fu, P. Ma, Z. Duan, X. Li, H. Lei, L. Chi, and Y. Li, Macromol Biosci **19**, 1800424 (2019).

O21. Doping of TiO_2 with different metals to enhance the performance of dye-sensitized solar cells

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Abstract

In this study, the TiO_2 semiconductor, used as a photoanode for efficiency enhancement in dye-sensitized solar cells, was doped with Zn, Cd, and Hg metals. The fabricated photoanodes were characterized using UV-Vis/DRS spectroscopy, Electrochemical Impedance Spectroscopy, and Linear Sweep Voltammetry. The efficiencies of DSSCs that used Zn/TiO_2 Cd/TiO_2 Hg/TiO_2 photoanodes were determined as 4.68, 2.89, and 0.47, respectively.

Introduction

Dye-sensitized solar cells first emerged in 1991 through the work of Grätzel and colleagues [1]. These cells are devices that have been developed by taking the photosynthesis event as an example and that absorb light, have a wide band gap, and provide electron transition in semiconductors [2].

It has been reported by researchers that different metals are doped into TiO_2 to prevent electron recombination between TiO_2 and I/I_3^- electrolyte during these processes [3]. TiO_2 was used as a semiconductor in this study due to its low cost, chemical stability and non-toxic properties [4]. Photoanodes were formed using TiO_2 nanoparticles with doped Zn, Cd and Hg elements, selected due to investigate doping effect of same group. Microwave-assisted hydrothermal method was used for the synthesis of different metal ions doped TiO_2. The photoanodes prepared with synthesized samples were sensitized with N719 dye.

Method

5 mL of titanium isopropoxide (TTIP) was added to 60 mL of deionized water containing 5 mL of 1 M NaOH solution, and then transferred to a teflon lined hydrothermal reactor after mixing. The same processes were used for the synthesis of metal-doped TiO_2 by supplementing the corresponding metal salts of Zn, Cd and Hg to the solution before adding TTIP at TiO_2/dopant = 100/1 mol ratios. Microwave oven in which placed hydrothermal reactors was operated for 45 min at 380 W microwave power and 100 °C. The resulting TiO_2 or metal ion doped TiO_2 precipitates were separated via centrifugation, washed three times with deionized water and ethanol and dried at 70 °C for 24 h. All samples were heat treated at 450 °C for 3 h to acquire anatase TiO_2.

Results and Discussion

In the UV-Vis-DRS spectra shown in Fig. 1a, it can be observed that Hg/TiO_2, Cd/TiO_2, Zn/TiO_2, and TiO_2 exhibit different reflectance values from each other. The fact that the reflectance values are different but not significantly distant from each other indicates the success of the doping process.

The J-V curves obtained from linear sweep voltammetry of DSSCs formed with photoanodes prepared with Zn, Cd, Hg doped TiO_2s and sensitized with N719 dye were given in Fig. 1b. The DSSCs efficiency values (ɳ) for the photoanodes prepared with Zn, Cd, Hg doped TiO_2s are 4.68, 2.89, 0.47, respectively.

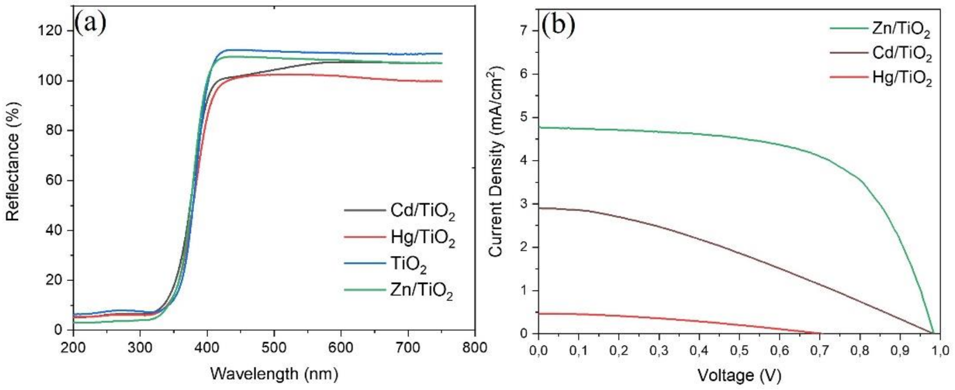

Figure 1. a) UV-DRS spectra of synthesized nanoparticles and b) J-V curves of DSSCs that were prepared with doped TiO_2 photoanodes

Considering the Bode and Nyquist diagrams in Fig. 2, Hg/TiO_2 showed much higher resistance than other doped TiO_2 nanoparticles. Electrochemical values obtained from electrochemical impedance spectroscopy can be seen in Table 1. It is understood from the calculated electron lifetime value that there is recombination due to large ionic radii of Hg^{2+} comparing to the Ti^{4+}. These larger ionic radii of Hg^{2+} might be cause large crystal defects. Therefore, there are more recombination centers for carried charges. Even though R_{CT2} value of Cd/TiO_2 is lower than Zn/TiO_2, efficiency is higher for Zn/TiO_2 photoanode. Similar to the Hg/TiO_2, Cd^{2+} ionic radii is higher than TiO_2. While lowest R_{CT2} value obtained for Cd/TiO_2, fill factor value is lower than Zn/TiO_2.

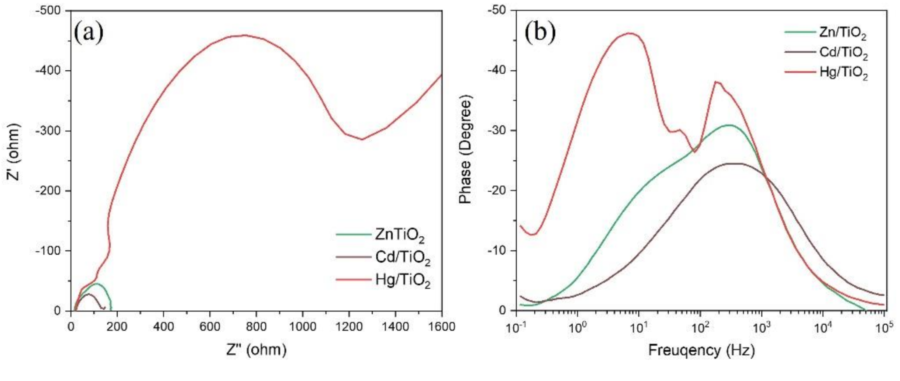

Figure 2. a) Nyquist and b) Bode plots of prepared DSSCs

Table 1. Electrochemical parameters obtained from EIS

Sample	R_S(Ω)	R_{CT1}(Ω)	R_{CT2}(Ω)	f_{max}(Hz)	$τ_e$(ms)

Zn/TiO_2	15,15	24,8	143,54	275,93	0,58
Cd/TiO_2	21,30	10,2	118,97	310,29	0,51
Hg/TiO_2	21,16	33.56	1095,85	6,85	23,24

Conclusion

Zn, Cd, Hg doped TiO_2 nanoparticles were synthesized via microwave-assisted hydrothermal method and used as photoanode material for DSSCs. Due to similarity of ionic radii of Zn^{2+} and Ti^{4+}, Zn/TiO_2 photoanode gave the highest efficiency value.

References:

[1] M. Grätzel, J. Photochem. Photobiol. C: Photochem. Rev., *4*(2), 145-153. (2003).
[2] T. Trupke, M.A. Green, P. Würfel, *J. Appl. Phys.*, *92*(7), 4117-4122. (2002).
[3] B. Roose, S. Pathak, U. Steiner, *Chem. Soc. Rev.*, *44*(22), 8326-8349. (2015).
[4] Z.D. Mahmoudabadi, E. Eslami, M. Narimisa, *J. Col. Interf. Sci.*, *529*, 538-546. (2018).

O22. Atomic system: the structuring mechanisms of atomic shells

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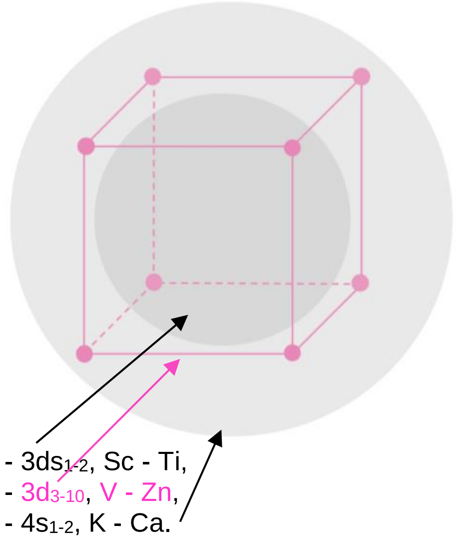
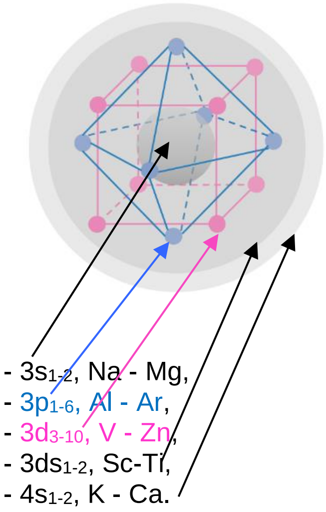
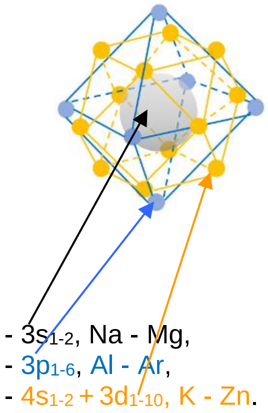
The structure of atoms has been described in this research work as an engineering system, by introducing some innovative elementary theoretical concepts such as:

- Identification of the structural roles of electrons; Subdivision into mobile electrons, who have the role of single or double protection and division of the shells (electrons s$_{1-2}$, d$_{1-2}$, f$_{1-2}$) and localized electrons, that can form *skeleton* electrons and *filling* electrons (p$_{1-6}$, d$_{3-8}$, f$_{3-14}$).
- Interpretation of the free electron pair not as a concentration of the electron cloud on one side of the nucleus (lone pair), but as a symmetrical distribution of the electron cloud on both sides [1]; Localized electrons so arranged find the equidistant positions from themselves and the nucleus, and form, according to their quantity in the shell, the symmetries attributable to the vertices of the Platonian solids [2] as octahedron, cube, icosahedron, but too the symmetries of cuboctahedron.

The table below illustrates some of the symmetries of the structuring of the 3d shell.

shell 3d *expanded*	shell 3d *condensed*	shells 3d+4s *hyper condensed*
		

Starting from sub-illustrate method with which the structuring of the atomic shells is interpreted, we want to analyze the following properties of the 3d series elements:

- metal and non -metal properties,
- high and low spin of shell structure,
- magnetic and paramagnetic properties of the complex of 3d series elements.

References

[1] J. Niewiadomska-Kaplar, *Modello ID Un nuovo approccio per l'interpretazione dei meccanismi di relazione tra gli atomi nelle molecole*, tabedizioni, Rome, p. 43-64 (2022).

[2] M. Cieślak-Golonka, J. Starosta, M. Wasilewski, *Wstęp do chemi koordynacyjnej*, Wydawnictwo Naukowe PWN, Warszawa, p. 21 (2010).

O23. Fabrication of dual responsive polymer microgel containing silver nanoparticles with catalytic and antibacterial activity

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Nanocomposites consisting of stimuli responsive microgels fabricated with metal nanoparticles have emerged as efficient, user friendly, recyclable and environment friendly catalysts and antibacterial agents. In this work, preparation of bare poly (N-isopropyl acrylamide-co-vinyl phosphonic acid) [p(NIPAM-co-VPA)] microgel by free radical polymerization and their fabrication with silver nanoparticles by in situ reduction is reported. The prepared bare and composite microgel was subjected to characterization with UV-Visible spectroscopy, Fourier transformation infra-red spectroscopy, X-ray diffraction, and Laser light scattering. The hydrodynamic diameters of the swollen microgel particles were found in the range of 66-82 nm and a small decrease was noted after the integration of silver nanoparticles. The catalytic potential was demonstrated in the chemical reduction of 4-nitrophenol (4-NP) and 2-nitrophenol (2-NP), eosin Y (EY), and methyl orange (MO) which were chosen as representatives of nitro compounds and dyes. The catalytic activity of the prepared nanocomposite was examined in the chemical reduction of 4-NP, 2-NP, EY, and MO with sodium borohydride in the aqueous medium. The thermodynamics of the catalytic reaction was analyzed by conducting the experiments at different temperatures and corresponding parameters such as activation energy, activation entropy change, activation enthalpy change, and Gibb's free energy were also calculated. The reduction rates of 4-NP, 2-NP, MO, and EY were calculated as 0.36, 0.24, 0.40, and 0.17 min−1, respectively. For evaluating the antibacterial potential, the prepared nanocomposite was tested against gram-positive bacteria [Staphylococcus epidermidis (ATCC: 14990)], and Gram-negative bacterial strains [Klebsiella pneumonia (ATCC: 4617), and Escherichia coli (ATCC-15224)]. The prepared nanocomposites showed activity against all the selected pathogenic strains with promising zones of inhibition of 17±0.82mm against Staphylococcus epidermidis and 15±0.91 against Escherichia coli and 15±1.52mm against Klebsiella pneumonia.

O24. Effect of Thiourea Concentration on Physical Properties of Sprayed Cu2MnSnS4 Thin Films

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Cu2MnSnS4 (CMnTS) thin films were deposited on soda lime glass substrates with different molar concentrations of thiourea using ultrasonic spray pyrolysis technique without sulfurization. The thiourea concentration was varied in order to investigate its influence on the properties of the CMnTS films and to determine the optimum concentration for pure CMnTS kesterite. As a result, the sample prepared at thiourea concentration of 0.25 M is the most suitable for depositing the high-quality CMnTS thin films. Characterizations of the structural, optical, and electrical properties of these films were studied by X-ray diffraction (XRD), Raman spectrometry, and UV–VIS absorption spectroscopy. X-ray diffraction and Raman spectroscopy analysis confirmed the formation of CMnTS tetragonal structure with preferential orientation along the (112) direction. Further, XRD reveals the appearance of a small peak, which are attributed to the secondary phases Cu2-xS and MnS. Optical measurements showed a high absorption coefficient towards the visible range (>104 cm−1) and the direct band gap decreased with decreasing thiourea concentration from 2.22 eV to 1.9 eV. The band gap broadening could be attributed to the secondary phase Cu2-xS for CMnTS. Electrical resistivity was measured by the four-point probe method. These experimental results revealed the best properties of the film that make it a suitable material for photovoltaic solar cells.

References

[1] MARCHIONNA, S., LE DONNE, A., MERLINI, M., et al. Growth of Cu2MnSnS4 PV absorbers by sulfurization of evaporated precursors. Journal of Alloys and Compounds, 2017, vol. 693, p. 95-102.
[2] YU, Jiejin, DENG, Hongmei, ZHANG, Qiao, et al. The role of sulfurization temperature on the morphological, structural and optical properties of electroplated Cu2MnSnS4 absorbers for photovoltaics. Materials Letters, 2018, vol. 233, p. 111-114.
[3] YU, Jiejin, DENG, Hongmei, TAO, Jiahua, et al. Synthesis of Cu2MnSnS4 thin film deposited on seeded fluorine doped tin oxide substrate via a green and low-cost electrodeposition method. Materials Letters, 2017, vol. 191, p. 186-188.

O25. Reshaping the perifollicular niche to combat Androgenetic Alopecia

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Androgenetic alopecia (AGA) is an extremely common disorder affecting 85% of men and 40% of women worldwide. It is mainly a genetically predetermined disorder characterized by excessive sensitivity to androgens, resulting in progressive and patterned thinning of scalp hair [1]. Current therapeutic options are limited to two United States Food & Drug Administration approved over-thecounter drugs, minoxidil and finasteride, which have drawbacks including partial hair regrowth, continuous usage requirement, and potential side effects. Hair transplant procedures offer a viable solution but are invasive, costly, and may have limited donor hair availability, leading to unsatisfactory outcomes.

Alternative approaches are urgently needed to address these limitations. The microenvironment around the hair follicles is a promising area of research, with great potential as an AGA sustainable treatment, as it plays a critical role in regulating hair follicle development, maintenance, and regeneration. Disruptions in the perifollicular niche, such as compromised blood supply and increased reactive oxygen species, significantly contribute to hair follicle dysfunction and subsequent hair loss [2, 3].

Given this, the present task is focused on developing a therapeutic approach comprising of stable biomimetic nanoformulations, named plateletmembrane

camouflaged nanoparticles. To obtain the platelet membrane, the process starts with the extraction of platelet-rich plasma (PRP) from whole blood samples. Once PRP is obtained, platelets are further separated and concentrated using additional centrifugation steps. After obtaining the platelet concentrate, freeze-thaw cycles are employed and used to disrupt the platelet cells and release their membrane components, followed by an isolation and purifying process. To reach the final biomimetic design, the extracted platelet membranes are fused with a poly (lactic-co-glycolic acid) (PLGA) core, due to its biocompatibility, biodegradability, and versatile drug loading. This PLGA core is produced by an optimized nanoprecipitation protocol and is loaded with melatonin. Melatonin is known for its impact on hair regrowth, but also, to its antioxidant properties, which is ideal to counteract ROS levels in the perifollicular niche [4, 5]. The fusion between the polymeric core and the platelet membrane is performed by optimized protocols of sonication, extrusion, or both combined. The preservation of critical platelet membrane proteins essential to this project is confirmed via western blotting, and the PLGA core loaded with melatonin is characterized in terms of size, polydispersity index, zeta potential, in vitro drug release, encapsulation efficiency, drug loading, and morphology.

The goal of this task is to obtain stable delivery systems for further incorporation within polymer-based microneedle patches. We plan to obtain stable biomimetic nanoparticles containing melatonin with high loading capacity, and an in vitro drug controlled release. As for further experiments, we plan to produce platelet-cloaked nanoparticle conjugated with the Vascular Endothelial Growth Factor (VEGF), to enhance angiogenesis in the perifollicular niche.

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References

[1] Chen, S.; Xie, X.; Zhang, G.; Zhang, Y. Comorbidities in Androgenetic Alopecia: A Comprehensive Review. Dermatol. Ther. (Heidelb). 12, 2233–2247 (2022).

[2] Staege, S.; Haslam, I.S.; Jadkauskaite, L.; Imre, L.; Hesebeck-brinckmann, J.; Jenkins, G.; Bhogal, R.K.; Lim, F.; Farjo, N.; Scha, M.; et al. Oxidative Damage Control in a Human (Mini-) Organ : Nrf2 Activation Protects against Oxidative Stress-Induced Hair Growth Inhibition. J. Invest. Dermatol. 137, 295–304 (2017).

[3] Chew, E.G.Y.; Tan, J.H.J.; Bahta, A.W.; Liu, X.; Lim, T.C.; Sia, Y.Y.; Heilmann, S.; Philpott, M.P.; Hillmer, A.M. Differential Expression between Human Dermal Papilla Cells from Balding and Non-Balding Scalps Reveals New Candidate Genes for Androgenetic Alopecia. J. Invest. Dermatol. 136, 1559–1567 (2016).

[4] Badajouni, A.; Reddy, M.; Rebecca, Z.; Raffi, J.; Phong, C.; Mesinkovska, N. Melatonin and the Human Hair Follicle. J. Drugs. Dermatol. 22, 260–264 (2023).

[5] Fischer, T.W.; Trüeb, R.M.; Hänggi, G.; Innocenti, M.; Elsner, P. Topical Melatonin for Treatment of Androgenetic Alopecia. Int. J. Trichology. 4, 236–245 (2012).

O26. Comparative analysis of kappa- and iota-carrageenan hydrogels for effective skin delivery

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Introduction:

Hydrogels exhibit extensive hydrophilic properties, forming three-dimensional polymeric networks [1]. Their remarkable biocompatibility with the human body makes them highly valuable materials in diverse fields such as pharmaceuticals, biomedicine, and cosmetics [2]. We produced hydrogels by combining synthetic (polyvinyl pyrrolidone, PVP) and natural (carrageenans, k-CRG or i-CRG) polymers. Obtained copolymers hydrogels were filled with transethosomes (TEs), which are nanocarriers with ultra-deformability and enhanced skin permeability properties [3].

This work investigates and compares the two types of hydrogels with and without TEs as potential vehicles for future skin delivery.

Methods:

The rheology (viscosity, thixotropy, shear rate, temperature stability) and morphology (SEM) evaluations of hydrogels were performed. The polymer structure was characterized by Fourier transform infrared spectrum (FTIR). The antioxidant activity of CRG-based hydrogels was analyzed by ABTS assay. Cell viability assays were carried out with HaCaT, and L929 cell lines. Quantifying cytokines. IL-4, IL-6, and THFα secreted by THP-1 differentiated macrophages performed via enzyme-linked immunosorbent assay (ELISA). Skin permeability was quantified based on fluorescent markers using Franz cell assays and visualized by confocal microscopy.

Results:

Based on rheological properties produced hydrogels showed storage stability for up to 10 weeks, were suitable for skin application, and had non-grease texture and uniform spreadability. i-CRG-based hydrogels demonstrated a thixotropic behaviour opposite to k-CRG. In the morphological point, the hydrogels displayed a porous 3D network silk-like structure formed by copolymer hydrogel (Figure 1).

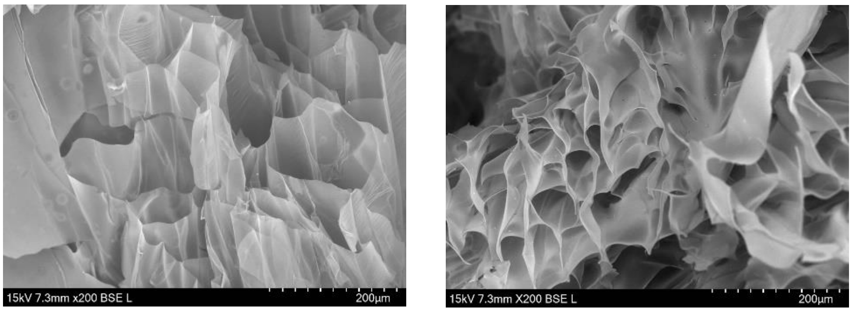

Figure 1 – SEM images of freeze-dried hydrogels (k-CRG – right, i-CRG – left side). Scale bar 200x

According to the FTIR data, we can confirm that i-CRG contains more sulfate groups than k-CRG, also PVP is miscible with CRG. i-CRG has higher antioxidant activity than k-CRG, which is correlated with a higher presence of sulfate groups. k-CRG-based hydrogels are less toxic for fibroblasts and keratinocytes. ELISA findings indicate that CRG didn't promote the secretion of pro-inflammatory (IL-6, THFα) cytokines. Moreover, the presence of CRG increased anti-inflammatory (IL-4) cytokines production. Porcine skin permeation assays demonstrated about 40% retention of hydrogels in the skin. Confocal microscopy showed the distribution of permeated hydrogels. In conclusion, produced CRG-based hydrogels are suitable vehicles for skin delivery, which have per se antioxidant and anti-inflammatory properties.

Acknowledgements:

This work received financial support from PT national funds (FCT/MCTES, Fundação para a Ciência e Tecnologia and Ministério da Ciência, Tecnologia e Ensino Superior) through grants UID/QUI/50006/2020. SCL thanks funding from FCT/MEC (CEECINST/00007/2021) financed by national funds. ZS thanks her for funding from FCT/MEC (2021.08549.BD). To all financing sources, the authors are greatly indebted.

References:

[1] A.I. Barbosa, T. Torres, S.A.C. Lima, and S. Reis, *Adv. Therapeutics*, **4** (2021).
[2] V.E. Santo, A.M. Frias, M. Carida, R. Cancedda, M. E. Gomes, J. F. Mano, and R. L. Reis Biomacromolecules, **10,** 6 (2009)
[3] R. Basto, R. Andrade, C. Nunes, S.A.C. Lima and S. Reis, *Pharmaceutics*, **13**, 11 (2021).

O27. Selecting a buffer layer for high-temperature carbon-assisted electrolysis cell with $SrFe_{0.75}Mo_{0.25}O_{3-\delta}$ anode

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The increasing global emphasis on clean and sustainable technologies has spurred a growing demand for hydrogen as a versatile energy carrier. One of the most promising pathways for hydrogen production is through water/steam electrolysis, although the high energy-demanding nature of the process has posed significant challenges. To address this, the concept of carbon-assisted electrolysis has emerged as a potential solution, offering the prospect of considerably lowering energy requirements while enhancing overall efficiency. A pivotal advantage lies in the fact that the introduction of carbon significantly reduces the Gibbs free energy necessary for the electrolytic reactions to occur. Specifically, the reaction $C + H_2O \rightarrow CO + H_2$ exhibits a notably reduced enthalpy change (ΔH) at elevated temperatures, with ΔH at 25°C being +31.14 kJ/mol. As the temperature surpasses 800 °C, the energy consumption of carbon-assisted electrolysis becomes merely one-fifth of that required by conventional water electrolysis at ambient conditions. This pivotal discovery underscores the potential of high-temperature operation in harnessing hydrogen from water sources with remarkable energy efficiency [1].

However, this innovation presents its own set of challenges. The utilization of carbon as a fuel at the anode necessitates the selection of an anode material that can maintain stability across an extensive range of oxygen partial pressures. Additionally, the chosen material must exhibit exceptional tolerance to impurities that might be present, particularly in coal-derived sources, as well as low resistivity to enable the high current densities necessary for practical applications. Strontium ferrite doped with molybdenum $SrFe_{0.75}Mo_{0.25}O_{3-\delta}$ was proposed as a highly suitable candidate meeting these demanding criteria. The $SrFe_{0.75}Mo_{0.25}O_{3-\delta}$ composition demonstrates acceptable electrical conductivity and notable stability under reducing conditions, even at oxygen partial pressures down to 10^{-20} atm [2]. These characteristics position it as a prospective electrode material for carbon-assisted electrolysis.

Nevertheless, a potential hurdle arises due to the interaction between $SrFe_{0.75}Mo_{0.25}O_{3-\delta}$ and yttria-stabilized zirconia (YSZ), a commonly employed electrolyte material. This interaction emphasizes the necessity of utilizing protective buffer layers to ensure optimal performance and longevity of the electrode. To address this challenge, the feasibility of employing fluorite-type $Ce_{0.8}Gd_{0.2}O_{2-\delta}$ and pyrochlore-type $Y_{1.8}Ca_{0.2}Ti_2O_{7-\delta}$ as buffer layers was thoroughly assessed. The investigation involved the fabrication of symmetric cells comprising YSZ electrolytes and $SrFe_{0.75}Mo_{0.25}O_{3-d}$ electrodes, with buffer layers applied through a spray-coating process. The entire assembly underwent sintering at 1500°C for 2 hours before application of electrode layers using a screen-printing technique. Subsequent sintering of electrodes at different temperatures (950°C, 1000°C, and 1050°C) with a controlled rate yielded electrode performance insights. The tests included chemical and thermomechanical compatibility assessment by XRD, microscopy (SEM/EDS), and controlled-atmosphere dilatometry. The electrochemical performance of symmetrical cells with different buffer layers and Pt gauze current collectors was investigated by electrochemical impedance spectroscopy at 600-850°C.

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References

[1] Ju, HyungKuk, Sukhvinder Badwal, and Sarbjit Giddey. Applied energy 231 (2018): 502-533.
[2] Merkulov, Oleg V., et al. Dalton Transactions 48.14 (2019): 4530-4537.

O28. Characterization of $CaVO_3$, $SrVO_3$ and $SrMoO_3$ perovskites as anode materials for biogas-fueled solid oxide fuel cells

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Significant attention has been drawn recently to rare-earth and alkaline-earth vanadates and molybdates due to their high potential as materials for electrochemical applications, particularly redox-reversible components for fuel electrodes of solid oxide fuel cells (SOFCs) [1-2]. In particular, $(Ln,A)VO_y$-derived components (where A represents an alkaline-earth metal cation) offer an essential advantage in the case of natural gas- and biogas-fueled SOFCs due to their anticipated resistance against carbon deposition and sulfur-containing impurities. The present study is focused on the comparative characterization of a series of perovskite-type compounds - $SrVO_{3-\delta}$, $SrMoO_{3-\delta}$ and $CaVO_{3-\delta}$ - as prospective anode components.

The ceramic materials were synthesized using a solid-state reaction route under controlled atmospheres. Special efforts were undertaken to design the synthetic procedure to prepare phase-pure perovskites. Ceramics samples for characterization were sintered between 1350-1500°C under reducing conditions. Crystal structure and microstructure of prepared materials were characterized by XRD and SEM/EDS. Thermomechanical compatibility with solid electrolytes was tested by controlled-atmosphere dilatometry. Electrical conductivity was measured as a function of temperature and oxygen partial pressure within the phase stability domain of the perovskite phase. High-$p(O_2)$ stability boundaries at relevant operation temperatures were determined in the course of the electrical measurements. The redox behavior on cycling between reducing and oxidizing atmospheres was assessed by conductivity relaxation, thermogravimetry and dilatometric studies combined with room-temperature XRD and microstructural inspection. The properties of materials are analyzed in terms of their applicability in SOFC anodes.

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References

[1] L. Adijanto, V.B. Padmanabhan, R. Küngas, R.J. Gorte, J.M. Vohs, J. Mater. Chem. 22 (2012) 11396.
[2] E.V. Tsipis, M.V. Patrakeev, V.V. Kharton, N.P. Vyshatko, J.R. Frade, J. Mater. Chem. 12 (2002) 3738.

O29. Exploring Yttrium-Doped Zirconate Stannate ($BaZr_{0.8-x}Sn_xY_{0.2}O_{3-\delta}$) proton-conducting electrolytes: Synthesis, characterization, and stability in CO_2 environment

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Barium stannates exhibit distinctive structural and chemical properties, making them excellent candidates for use in proton ceramic electrolyte applications. This study focuses on optimizing the composition and structure of barium stannate electrolytes to enhance their performance [1-3]. The compositions were synthesized through solid-state reactions, and the X-ray diffraction (XRD) analysis confirmed the formation of a pure phase across the entire compositional range after sintering at 1550 °C. It was observed that the relative density increases with the introduction of tin (Sn) doping, leading to enhanced grain growth, as evidenced by scanning electron microscope (SEM) images. Furthermore, the stability of the doped composition (x=0.4) was evaluated in a humidified carbonaceous environment at 600 °C, demonstrating outstanding stability. This research underscores the significant potential of barium stannates, particularly as electrolytes in environments containing CO_2, potentially opening up a novel, sustainable, and efficient pathway for CO_2 utilization.

Acknowledgments

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References

[1] Y. Wang, A. Chesnaud, E. Bevillon and G. Dezanneau, *Solid State Ionics*, 2012, **214**, 45–55.
[2] I. A. Zvonareva and D. A. Medvedev, *J. Eur. Ceram. Soc.*, 2023, **43**, 198–207.
[3] L. Putilov and V. Tsidilkovski, Materials 2022, **15**, 4795.

O30. The influence of ultrasmall palladium nanoparticles (Pd NPs) PEGylation on their radiosensitizing effect in simulated proton radiotherapy of glioblastoma multiforme (*in vitro* model)

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The increasing number of cancer cases every year necessitates finding new strategies for effective treatment of this disease. Traditional treatment methods are often unsatisfactory and may cause numerous side effects [1]. A relatively new method of treating cancer is proton radiotherapy. This type of radiotherapy, compared to classic radiotherapy (using X-ray or gamma rays) allows for larger accuracy in irradiating the tumor. For protons, the maximum therapeutic dose (the so-called Bragg peak) occurs at a specific depth depending on the beam energy, and not on the patient's skin (as in the case of photon radiotherapy). Such a favorable distribution of the proton dose enables, in particular, the use of this type of radiotherapy to irradiate tumors located deep in the body (e.g. gliomas) [2]. Additionally, the effect of radiotherapy can be increased by adding the so-called radiosensitizers which, as a result of interaction with protons, generate (among others) reactive oxygen species, enhancing the effect of therapy and at the same time enabling a reduction in the total radiation dose [3]. As part of this research, we obtained radiosensitizers in the form of ultrasmall (~ 3 nm) spherical palladium nanoparticles (Pd NPs). These Pd NPs are an effective alternative to the more commonly used gold nanoparticles (Au NPs), but the cost of producing the latter is much higher [4]. However, due to the high cytotoxicity of unmodified nanosystems, they should be appropriately biofunctionalized [5]. For this purpose, we attached poly(ethylene glycol) to the surface of the Pd NPs. This modification results in masking the toxicity of the nanomaterials. Then, the therapeutic effect of the pre-synthesized PEG-(un)modified Pd NPs was tested on two glioblastoma cell lines (LN229 and U118 cells). These cells were cultured with non-toxic concentration of nanosystems and then irradiated by a proton beam with a therapeutic dose of 2 Gy, typical for irradiation of gliomas. A number of biological tests (MTS test, flow cytometry, clonogenic assay) were used to evaluate the effectiveness of these NPs. Study results showed a more satisfactory radiosensitizing effect when using functionalized nanosystems compared to unmodified Pd NPs.

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References

[1] R. L. Siegel, K. D. Miller, N. S. Wagle, A. Jemal, *CA Cancer J Clin*, **73**, 17-48 (2023).
[2] I. Chambrelant, J. Eber, D. Antoni, H. Burckel, G. Noel, R. Auvergne, *Radiation*, **1**, 218-233 (2021).

[3] C-Y. Lo, S-W. Tsai, H. Niu F-H. Chen, H-C. Hwang, T-C. Hsiao, J-W. Liaw, *ACS Omega*, **8**, 17922-17931 (2023).

[4] Y-W. Jiang, G. Gao, H-R. Jia, X. Zhang, X. Cheng, H-Y. Wang, P. Liu, F-G. Wu, *Langmuir*, **36**, 11637 (2020).

[5] O. Długosz, K. Szostak, A. Staroń, J. Pulik-Prociak, M. Banach, *Materials (Basel)*, **13**, 279 (2020).

O31. Plasma electrolytic oxidation synthesis of TiO_2/CuO heterostructures and characterization for photoanode applications

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In the renewable energy field, conversion of solar light into electrical or chemical energy is considered essential in order to move towards a green energy economy. Solar energy can be harnessed by driving photoelectrochemical (PEC) reactions such as water splitting or pollutant oxidation with the use of photocatalytic materials. In this study TiO_2 films were synthesized electrochemically by a procedure, called plasma electrolytic oxidation (PEO). Different thickness and morphology were obtained by tuning synthesis conditions (electrolyte, duration, current density and voltage) (Fig. 1a, b). TiO_2/Cu_xO heterostructures were synthesized with a Cu^{2+} precursor added to the solution. The obtained TiO_2 and heterostructured films were characterized for their structural (XRD, XPS, FTIR), and optical (UV-vis diffuse reflectance spectroscopy) properties.

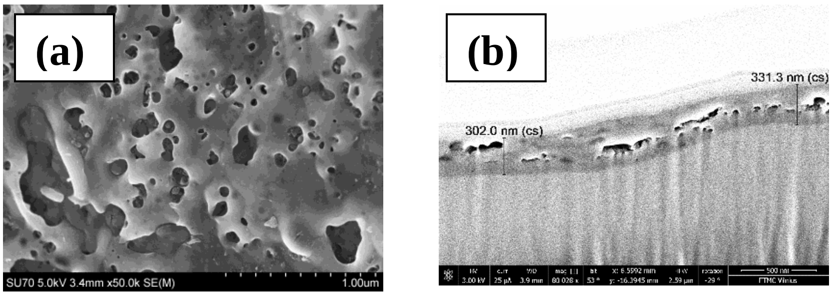

Fig. 1. *(a) Surface morphology of TiO_2 film, synthesized by PEO; (b) FIB cross-section morphology of same film;*

The films show good PEC water splitting activity in alkaline media with a 365 nm LED light source. The obtained photocurrent depends on the maximum synthesis voltage, and heterostructuring with CuO lowered the band gap and improved the PEC performance of the films. Surface electron-hole recombination was evaluated by intensity modulated photocurrent spectroscopy (IMPS), and the effect of a hole scavenger (methanol) was evaluated.

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O32. Electrolytic rhenium alloys with iron-group metals: synthesis, properties and applications

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Electrolytic alloys of nickel, cobalt and iron with rhenium are promising modern materials possessing a wide range of valuable properties that allow them to use even in extreme conditions. Depending on the ratio of metals in the alloy, these materials can be used as anti-corrosion, hard and wear-resistant coatings, soft magnetic materials for hermetic contacts, magnetic microsensors, in information recording devices, as catalysts, and in the devices where stability of properties at high temperatures is very important, e.g. in the aerospace and nuclear industries.. Analysis of the electronic configuration of metals shows that the highest catalytic effect on the hydrogen evolution reaction (HER) should be observed when one metal has d^4-d^5-, and another d^6-d^8-electron configuration. Therefore, rhenium alloys can be served as a cathode for HER.

The intensive study of Re-alloys electrodeposition started in 1990s: up to now only 76 papers published in journals having impact-factor, and only ~50 papers deal with Re-alloys with iron-group metals. The main attention is paid for Ni-Re alloys, some results are published on Co-Re alloy, whereas research on Fe-Re alloys has been scarce.

We are developing production methods that use stable, non-toxic electrolytes. The chemical composition, morphology and structure of the surface of polymetallic coatings produced by the electrochemical deposition from various baths (sulphamate, citrate, citrate-pyrophosphate), have been synthesized and studied. The main regularities of the influence of electrolysis conditions and mechanism of electrochemical synthesis (induced and classic) rhenium alloys, on the qualitative and quantitative composition of deposits. It was determined that the electrocatalytic activity is qualitatively proportional to the refractory metal content in alloys.

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O33. Local properties of mild steel

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Mild steel is a type of carbon steel that contains a low level of carbon (between 0.05% and 0.25% of carbon by weight). The combination of materials that create low carbon steel gives the metal particular qualities (conductivity, ductile, machinable, weldable, magnetic) that make it suitable for a variety of industrial projects. During the operation of metal structures, many different types of defects occur that affect the properties of the materials. Mechanical deformations and mechanical stability are most important for metals. So, for the successful use of these materials, it is necessary to know how these mechanical deformations (local dents, defects, scratches) affect they physical properties. These defects have local nature and for investigation effect of these defects need to use local methods too. AFM (atomic force microscopy), nanoindentation, micro-scratching techniques have been successfully used to investigate the physical properties of materials at the nanoscale levels.

In this work we investigated local properties of mild steel (M T Metalworks Brynteg, United Kingdom) by AFM methods after local mechanical deformation (nanoindentation, micro-scratching). By kelvin probe force microscopy (KFM) surface potential after deformation changed on -300 mV in deformed area with additional modulation of surface potential correspond to local surface shape (bending). In these deformed areas decreasing conductivity is detected by spreading resistance imaging. Some correlations mechanical deformation and magnetic domain distribution and local friction properties was found by magnetic force microscopy (MFM) and friction force microscopy (FFM) after nanoindentation. So, AFM local measurements of mild steel showed clear correlations between mechanical deformations and conductivity, magnetism, charge distribution in the deformation area directly and at distances of up to several microns.

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

O34. Revealing surface exchange kinetics on the new layered barium cobaltite electrode for Protonic Ceramic Cells (PCCs)

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Protonic Ceramic Cells (PCCs) represent promising energy storage and conversion devices for operation at the intermediate temperature range of 500 °C to 700 °C, where a wide range of industrially important hydrogenation/de-hydrogenation reactions can occur. However, the widespread adoption of this technology depends on further developing high-performance electrode materials with enhanced chemical compatibility with common proton ceramic electrolytes. Hence, we here studied a new cobaltite material, $Ba_2Co_9O_{14}$ (BCO), and its potential role as an oxygen electrode in PCCs. BCO was found to be chemically stable with a $BaZr_{0.852}Y_{0.148}O_{3-\delta}$ (BZY15) electrolyte up to 900 °C in ambient air, as shown by X-ray diffraction studies. Electrochemical impedance spectroscopy measurements were applied to a symmetrical cell configuration of a BCO electrode and a BZY15 electrolyte substrate. Data was corrected to account for the electronic short-circuiting through the electrolyte – a drawback that leads to a significant underestimation of the electrode polarization resistance. Hence, a proper equivalent circuit model was applied to the data, revealing that the electrode kinetics is rate-limited at the electrode-electrolyte interface due to the relatively low ionic conductivity of the BCO phase – a factor that is concurrent with the absence of significant changes in the oxygen nonstoichiometry/water uptake of BCO samples measured by thermogravimetric experiments. Overall, the BCO electrode offers polarization resistances that are comparable to that from state-of-the-art oxygen electrodes in similar conditions while also being chemically stable. This work introduces a new intergrowth series of cobaltite-based electrodes for potential application in PCCs, where the current lack of suitable oxygen electrodes presents an exciting avenue for exploration.

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O35. Detection of leakages in closed circuits using luminescent nanoparticles as optical probes

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The purpose of this work is to develop a route for the detection of leakages in closed circuits, using luminescent and biocompatible nanoparticles as optical probes. To accomplish this, an experimental testing platform is being developed where nanoparticle powders dispersed in a gas will be injected into a quartz tube, simulating its trajectory in a pipeline. Cracks of different sizes within the quartz tube will be intentionally promoted to simulate local leakages. The system uses a Venturi eductor to disperse the nanoparticles in a simple and effective way. Compressed air is injected in one end of the eductor and, through the increase of the air velocity near the constriction area, the particles are sucked into the system and aerosolized in the expansion section. To obtain a stable and measurable luminescent signal from the nanoparticles, it is necessary to use an appropriate excitation light source. Light-emitting diodes are the most suitable option not only due to their high luminous flux but also due to the narrow emission wavelength, which can be specifically tailored to maximize the excitation of the nanoparticles. The optical detection is performed with an imaging system that includes cameras with a high quantum efficiency over the spectral range of the nanoparticles' emission, an optical sensor with a large number of pixels in order to be able to produce high-resolution images, a good dynamic range to enable the detection of big and small holes (higher and lower intensity signals, respectively) simultaneously, a small readout noise to detect low-intensity emission signals, and a data interface allowing control of the camera parameters with user-friendly software. Preliminary tests using this apparatus have shown very promising results at a laboratory level, revealing a huge potential for scaling up a similar system for industrial applications.

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O36. Iron electrowinning as a sustainable steelmaking technology: case studies

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Conventional steel manufacturing relies on carbothermal reduction of iron ores to produce iron metal, contributing up to approximately 9% of global CO_2 emissions [1]. With the growing global demand for steel, the decarbonization of the steel industry has become a major concern. Iron electrowinning from iron oxide suspensions in alkaline media has been explored over the past decades. This technology operates at a lower temperature (~100 °C) and generates hydrogen and oxygen gases as by-products, offering potential energy savings (6 GJ/ton of Fe) compared to the conventional steelmaking [2,3]. This study provides an overview of this technology progress, drawing from literature and case studies conducted by the authors.

Hematite-based powders and/or previously processed ceramic cathodes were used for case studies. To mitigate the unpredictable effects of complex compositions, the direct use of iron ores and iron-rich waste as raw materials was avoided. Instead, controlled additions of Al-Mg oxides in an iron oxide matrix enabled to assess the potential impact of non-conductive contaminants during the electroreduction of iron oxide to Fe. The electrochemical tests were performed in NaOH electrolytes (10 M) at 80-90 °C, with a Pt wire as a counter electrode and a reference electrode of Hg|HgO|NaOH (1 M). A PGSTAT302N potentiostat was used for chronoamperometry and cyclic-voltammetry studies. Combined XRD/SEM/EDS studies confirmed iron formation even with added impurities. Lower efficiencies (<30%) were observed when Al-Mg contaminations were added. However, when using lower load of contaminants (~7 wt%) or purely hematite, higher efficiencies were attained (>70%). This technology holds promise for a greener steelmaking future, as demonstrated by a recent pilot plant constructed by ArcelorMittal (France). It may represent a transformative shift in the metallurgy sector, with potential integration into intermittent renewable energy sources on the horizon.

References

[1] E.A. Mousa, *Metall. Mat. Eng.*, ***25**,* 69–104 (2019).
[2] J. de Beer, Potential for Industrial Energy-Efficiency Improvement in the Long Term, Springer, Utrecht (2000).
[3] A. Allanore, H. Lavelaine, J. P. Birat, G. Valentin, and F. Lapicque, *J. Appl. Electrochem.*, **40**, 1957–1966 (2010).

O37. Waste Heat Harvesting Using Calcium Cobaltite and Calcium Manganite-Based Thermoelectric Modules

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As the world's population is increasing rapidly, the necessity for energy is growing up by alarming rate. Given the limitation of conventional energy sources and their detrimental impact on global warming due to CO_2 emissions, finding alternative environmentally friendly energy sources is crucial. Furthermore, since more than 65% of the energy used in different sectors is wasted in the form of heat, there is a substantial and ongoing research effort in the area of thermoelectric materials. This research is driven by the potential of thermoelectric materials to efficiently convert heat directly into electricity, making them a promising technology for energy recovery [1].

Within this investigation, we present the fabrication and characterization of a thermoelectric module utilizing p-type Sr-doped calcium cobaltite ($Ca_3Co_4O_9$) material, and n-type Ce-doped calcium manganite ($CaMnO_3$) one [2]. These materials have demonstrated promising thermoelectric properties, making them suitable candidates for applications in waste heat recovery and the generation of sustainable energy.

For both types of precursors, we employed the attrition milling process, which offers a significant reduction in thermal processing time. The p-type material was prepared using hot pressing to achieve dense pellets, using the procedure previously described [3], while the n-type materials were sintered [2]. Subsequently, we conducted measurements of various thermoelectric properties, including the Seebeck coefficient, electrical conductivity, and thermal conductivity, for both compounds. These prepared legs were then assembled into a thermoelectric module pattern using the electrical series-thermal parallel configuration, with silver paste as a precursor for electrical interconnections. Finally, the module was characterized using a home-made system, cooling the cold side at about 18 ºC using a flowing water circuit, and heating the hot side to temperatures between 200 and 900°C.

The maximum power that could be achieved for this module is around 0.12 W at 900℃ with the temperature gradient of 463℃. The results demonstrate the potential of these thermoelectric modules to convert heat into electricity efficiently. This research contributes to the ongoing efforts in developing advanced materials for energy conversion and highlights the promise of calcium cobaltite and calcium manganite-based thermoelectric modules in addressing the global energy sustainability challenge.

Acknowledgements:

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References

[1] D. Champier, *Energy Convers. Manag*., **Volume**. **140**, pp. 167–181,(2017).

[2] A. Sotelo, P. Amirkhizi, O. J. Dura, G. García, A. C. Asensio, M. A. Torres, M. A. Madre, A. Kovalevsky, Sh. Rasekh, *Ceram. Int*. (2023) (Accepted).

[3] M. A. Torres, G. Garcia, I. Urrutibeascoa, M. A. Madre, J. C. Diez, A. Sotelo, *Sci. China Mater*. **Volume 62**, 399-406 (2019)

O38. Laser Floating Zone processing of $SrTiO_3$ and TiO_2 -based thermoelectrics

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Energy consumption is expected to continue rising, and thus, the need for more renewable and efficient energy sources is essential to ensure energy demands are reached in a sustainable way, without environmental degradation and/ or over-reliance on finite resources [1]. It is necessary to develop green energy production methods and energy-efficient technologies. Thermoelectric (TE) energy harvesting stands as a potential solution to improve the efficiencies across various high-temperature industries, ultimately resulting in efficiency improvements [2]. However, traditional TE are not suited for high temperatures or harsher environments; therefore, suitable and highly performing TE materials are necessary [3]. Oxide TE oxides are usually characterized by high chemical and thermal stability and are expected to be a candidate for this kind of applications [4]. Nevertheless, most oxides are not suited for TE applications, showing low ZT values when compared with traditional TE. Yet, by designing new compositions and micro-/nanostructures, while involving new processing techniques leading to unique microstructural and electrical properties, can result in increases in TE oxide performance [5]. Promising families of oxides suitable for TE applications include the titanates, namely $SrTiO_3$ and TiO_2. These oxides are very sensitive to redox and processing conditions, resulting in flexibility towards tuning of the electrical properties [6,7]. $SrTiO_3$ -based TE are among the most promising oxide TE, with a composite composition, STN + 0.5% reduced graphene, achieving a ZT value of 1.42 at ˜750 ºC [8]. Titanium dioxide processed at high pressure and high-temperature, combined with engineering of lattice defects, showed in an overall improvement of its thermoelectric properties, reaching a maximum ZT value of 0.33 at 700 °C for the $TiO_{1.76}$ [9]. This work focuses on a new approach for processing $SrTiO_3$ and TiO_2 -based TE materials by using the Laser Floating Zone (LFZ) technique. The LFZ processing offers several advantages for TE applications, like high density, uniform distribution of the cations composition in the melt, tunable phase formation and cation distribution controlled by the cooling rate, as well as slightly reducing conditions during laser growth [6]. This study analyzes and characterizes the relevant effects of LFZ processing on the structure, microstructure and thermoelectric performance of the $SrTiO_3$ -based and TiO_2 -based materials. The results indicate the ability to prepare these materials by LFZ, resulting in mechanically strong fibres with adequate electrical and TE properties. An annealing after LFZ processing was also employed in the $SrTiO_3$ samples, resulting in a considerable increase in electrical conductivity and relatively high power factor values, derived from the further reduction and consequent charge carrier generation, as well as phase stabilization.

References

[1] T. Ahmad and D. Zhang, “A critical review of comparative global historical energy consumption and future demand: The story told so far,” *Energy Reports*, vol. 6, pp. 1973–1991, Nov. 2020, doi: 10.1016/j.egyr.2020.07.020.

[2] J. He, Y. Liu, and R. Funahashi, “Oxide thermoelectrics: The challenges, progress, and outlook,” *J. Mater. Res.*, vol. 26, no. 15, pp. 1762–1772, 2011, doi: 10.1557/jmr.2011.108.

[3] F. P. Carreira, N. M. Ferreira, and A. V. Kovalevsky, “Laser processing as a tool for designing donor-substituted calcium manganite-based thermoelectrics,” *J. Alloys Compd.*, vol. 829, p. 154466, 2020, doi: 10.1016/j.jallcom.2020.154466.

[4] G. Ren *et al.*, “High Performance Oxides-Based Thermoelectric Materials,” *Jom*, vol. 67, no. 1, pp. 211–221, 2015, doi: 10.1007/s11837-014-1218-2.

[5] X. L. Shi *et al.*, “SrTiO3-based thermoelectrics: Progress and challenges,” *Nano Energy*, vol. 78, no. August, 2020, doi: 10.1016/j.nanoen.2020.105195.

[6] A. V. Kovalevsky *et al.*, “Redox engineering of strontium titanate-based thermoelectrics,” *J. Mater. Chem. A*, vol. 8, no. 15, pp. 7317–7330, 2020, doi: 10.1039/c9ta13824b.

[7] Y. Fan *et al.*, “Preparation of monophasic titanium sub-oxides of Magnéli phase with enhanced thermoelectric performance,” *J. Eur. Ceram. Soc.*, vol. 38, no. 2, pp. 507–513, 2018, doi: 10.1016/j.jeurceramsoc.2017.09.040.

[8] M. Acharya, S. S. Jana, M. Ranjan, and T. Maiti, “High performance (ZT>1) n-type oxide thermoelectric composites from earth abundant materials,” *Nano Energy*, vol. 84. 2021, doi: 10.1016/j.nanoen.2021.105905.

[9] H. Liu *et al.*, “High-thermoelectric performance of TiO 2-x fabricated under high pressure at high temperatures,” *J. Mater.*, vol. 3, no. 4, pp. 286–292, Dec. 2017, doi: 10.1016/j.jmat.2017.06.002.

O39. Perovskite thin films: Optoeletronic properties

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The climate changes and geopolitical tensions highlight the urgency of replacing fossil energy sources with renewable ones. In this context, the enormous solar power provided by the Sun to the Earth every day, which can be exploited sustainably for electricity production, is of great importance. The development of photovoltaic technologies is essential to increase the power conversion efficiency of these types of devices. Given the prevailing dominance of silicon in the photovoltaic market, adding perovskite cells to silicon photovoltaics to manufacture tandem photovoltaic devices with augmented efficiency emerges as a rational and promising path, since in the last decade perovskite-based solar cells attained a power conversion efficiency record of about 25.73 % [1]. Hybrid organic-inorganic perovskites such as $MAPb(I_{1-x}Br_x)_3$ have been investigated due to their excellent direct and tunable bandgap, strong light absorption, and high charge carrier mobility characteristics. Depending on the x value, the bandgap values vary between 1.59 eV (x=0) and 2.31 eV (x=1) [2].

In this work, a study was carried out on the optical properties of perovskite films with different compositions (x=0, 0.66, 1) using the photoluminescence technique to study the radiative and non-radiative recombination mechanisms. In particular, the dependence of luminescence on excitation power and temperature was analyzed. The stability of the films was also investigated. It was observed that luminescence strongly depends on these experimental parameters and the stability of the films under optical excitation was shown.

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References

[1] J. Park, J. Kim, H.-S. Yun, M. J. Paik, E. Noh, H. J. Mun, M. G. Kim, T. J. Shin and S. I. Seok Nature 616:724-730, 2022.
[2] R Singh, M Parashar, S Sandhu, K Yoo and J J Lee. Solar Energy, 220:43-50, 2021.

O40. The effects of black tea extracts on the corrosion inhibition of mild steel in acidic solution

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It was examined to evaluate the effectiveness of extracted tea leaves as the green corrosion inhibitor that contains mild steel in acidic solvents. The test specimens were dissolved in an acidic solution with different concentrations of the extracted tea leaves. After 3 hours of immersion, the corrosion rate (CR) was measured. The results showed that a concentration of 1000 mg/l caused a significant inhibition in corrosion rate as compared to control. To see how black tea (BT) extract affected mild steel corrosion in 1 M HCl, it was subjected to a loss of weight procedure. The corrosion level and the inhibitor's performance were examined at five different BT extract concentrations that included 0.4, 1 , 1.4 , 2, and 2.4 g/l. According to the findings, an increase in BT concentration at every temperature decreased CR. As a result of the rise in kinetic activities of the metal surface interface, typically, temperature elevation leads to an increase in CR at every concentration of BT extract. The study's findings showed that adding 2.4 g/l of inhibition efficiency resulted in a temperature of 323 K, resulting in 84.95% inhibition efficiency. The small activation energy (Ea) of 8.74 and 11.45 kJ/mole reflected the barrier layer properties of BT extract and its chemical interactions on mild steel surfaces. The thermodynamic parameter revealed the spontaneous interaction between BT extract species and steel surface as k_{ad} rose from 0.929 to 1.728 $(g/l)^{-1}$.

O41. Metalens Magic-Shaping the Future of Nanostructure Probing

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Abstract

Metalenses, a groundbreaking innovation in the field of optics, promise to revolutionize imaging, communication, and sensing applications. Unlike traditional lenses, metalenses are ultrathin, flat, and comprised of subwavelength nanostructures, enabling them to manipulate light in unprecedented ways. Here, we provide an overview of metalenses+, including their working principles, design, and diverse applications.

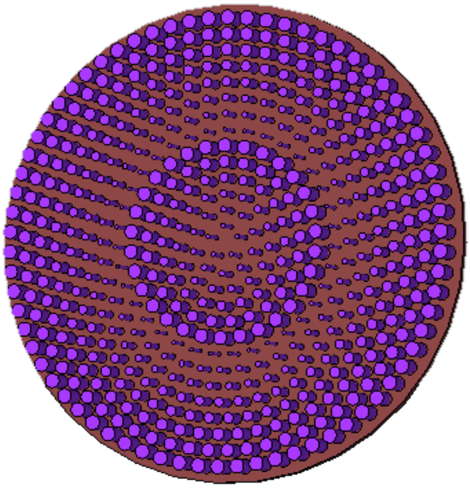

Fig: 3D view of Metalens

Introduction

Metalenses leverage the principles of nanophotonics to control the phase and amplitude of incoming light, enabling the precise manipulation of light waves. By relying on metasurfaces, which consist of arrays of nanostructures, metalenses can bend, focus, and shape light with extraordinary efficiency. Beyond imaging, metalenses find applications in augmented reality, virtual reality, and holography, where their compactness and ease of integration into optical systems offer transformative capabilities.

Design and Methodology

The design of metalenses involves creating a metasurface by arranging the optimized meta-atom in a specific pattern. The phase imparted by each meta-atom is calculated using the formula [1]:

$$\varphi = \frac{2\pi}{\lambda}\left(\sqrt{x^2 + y^2 + f^2} - f\right)$$

where λ is the wavelength of incident light, f is the focal length and x,y denotes the position of the meta-atom from the centre of the metalens. The analysis of the metalens is carried out using the Finite-Difference Time-Domain (FDTD) method.

Results and Discussion

Metalenses, designed through careful unit cell optimization exhibit exceptional performance in focusing and manipulating light. These metalenses exhibit exceptional performance in focusing and manipulating light, achieving high-resolution imaging, reduced aberrations, and customized functionalities. Their recent applications in achromatic focusing [2] and optical fibers further expand their potential.

References

[1] Arbabi A, Horie Y, Bagheri M, Faraon A. Dielectric metasurfaces for complete control of phase and polarization with subwavelength spatial resolution and high transmission. Nat Nanotechnol. 2015;10

[2] Yu, B., Wen, J., Chen, X. and Zhang, D., “An achromatic metalens in the near-infrared region with an array based on a single nano-rod unit,” Appl. Phys. Express 12(9) (2019).

O42. Analysis and measurements of the properties of light through Photonic crystal Fibers

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Abstract

Photonic Crystal Fibers are micro-structured optical fibers that are based upon a single material in which there are air holes running through the entire length of the fiber, hence it is also called the holey structure. The holey structure has got a periodic arrangement in the material and a break in the periodicity of the holes is the localized core of the fiber. The study of photonic crystal fibers has gained great attention over the past few years and the way holey fibers trap light, due to the large refractive index contrast between the holes and the solid background, make them unique. Microstructured optical fibers (MOFs) represent a revolutionary advancement in optical communication and sensing technologies, offering unique properties that transcend the limitations of traditional optical fibers.

Introduction

MOFs are characterized by an intricate pattern of air holes or voids that run along the length of the fiber, altering its optical properties [1]. The design principles involve tailoring the size, shape, and arrangement of these microstructures to achieve specific optical characteristics, such as dispersion control, birefringence, and enhanced light guidance. This level of customization enables MOFs to address diverse application requirements.

The fabrication of MOFs involves specialized techniques, including stack-and-draw, chemical vapor deposition, and photonic crystal fiber methods. These methods allow for precise control over the microstructure dimensions, ensuring reproducibility and reliability in mass production. Advances in fabrication technology have enabled the development of MOFs with varying core structures, such as solid-core, hollow-core, and suspended-core designs, each catering to specific applications.

Measuring Capabilities

Microstructured optical fibers offer a range of measurement capabilities, making them indispensable in diverse fields. Their unique properties enable efficient light coupling, high nonlinearities, and enhanced sensitivity to external factors. MOFs find applications in sensing technologies, such as temperature, strain, and refractive index sensing. Additionally, their ability to guide light in air channels allows for gas sensing, making them suitable for environmental monitoring and industrial applications.

The measurement capabilities of MOFs extend to nonlinear optics, enabling the generation of new frequencies through processes like four-wave mixing and supercontinuum generation. These capabilities open avenues for the development of compact, high-performance light sources for applications in telecommunications and spectroscopy.

In conclusion, microstructured optical fibers represent a paradigm shift in optical communication and sensing. Their design flexibility, coupled with advancements in fabrication techniques, has unlocked a plethora of measurement capabilities. From tailored dispersion control to nonlinear optical processes, MOFs continue to drive innovations across a spectrum of applications, promising a future of enhanced optical technology [2].

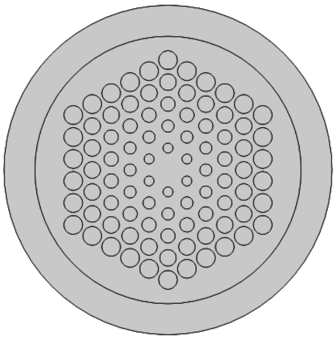

Fig1: Design of a microstructured fiber

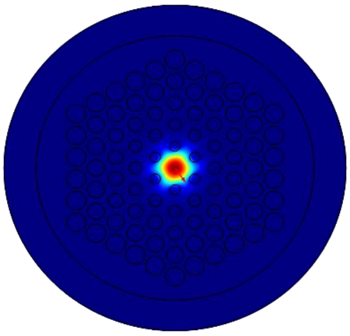

Fig2: Confinement of light in the fiber

Result

Various interesting phenomena are shown by the light-matter interaction in the photonic crystal structures. Microstructured Optical fibers have huge applications in the measurement of important characteristics of light, like dispersion [3], confinement loss, nonlinear effects, etc. They are also widely used as sensors for sensing blood glucose level, presence of gases in atmosphere, covid infectants, temperature, electric and magnetic fields etc, with a good accuracy. These properties are not only easily measured but as per the need the fiber can be designed with ease just by varying the size of the holes, the pitch or the number of layers to get better results.

References

[1] Russell. P, (2003), “Photonic crystal fibers”, Science;299(5605):358-62
[2] Varshney, Shailendra K., Singh M. P. and Sinha R. K, (2003), "Propagation Characteristics of Photonic Crystal Fibers" *Journal of Optical Communications*, vol. 24, no. 5, pp. 192-198.
[3] Song Gao, Xiaoyi Bao (2020), “Chalcogenide Taper and Its Nonlinear Effects and Sensing Applications”, iScience, Volume 23, Issue 1, 100802, ISSN 2589-0042.

O43. Degradation of methylene blue using TiO_2/reduced graphene oxide nanocomposite by advanced oxidation process

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Water contamination is one of the large serious environmental problems, as a wide range of hazardous substances are increasingly released into the water courses. The discharge of effluents from the textile and dyeing industries has been a worldwide concern. These toxic pollutants exhibit high toxicities and thus constitute serious threats to all living organisms. It is crucial to develop an efficient method for industrial wastewater treatment [1], [2]. One of the most promising methods for wastewater treatment is semiconductor-based heterogeneous photocatalysis. Titanium dioxide (TiO_2) is a promising semiconductor for the removal of various toxic pollutants due to its stability, low cost, non-toxicity, and corrosion resistance. However, there are numerous challenges limiting its practical applications, including poor adsorption capacity, high recombination rate of the photo-induced charge carriers, and wide band-gap energy (anatase ~3.2 eV). One of the approaches to overcome its limitations, enhance the photocatalytic efficiency, and activate visible light absorption is anchoring with graphene-based materials [3]. TiO_2@graphene-based nanocomposites are considered one of the most novel and effective approaches in the field of photocatalysis for their structure, large specific surface area, extraordinary electron mobility, high chemical stability, and electrical conductivities. Moreover, TiO_2@graphene-based nanocomposites enhance the adsorption ability and the photocatalytic performance in the new generation photocatalysts [4].

To take advantage of Solar illumination for its photodegradation, TiO_2/reduced graphene oxide (TiO_2@rGO) nanocomposites with different GO contents (4, 8, and 16 wt%) were synthesized using hydrothermal method followed by calcination treatment and characterized by X-ray powder diffraction (XRD), scanning and transmission electron microscopy (SEM/TEM), UV-vis diffuse reflectance spectroscopy (DRS) and Raman spectroscopies. Additionally, their specific surface areas (S_{BET}) and pore volume were determined. The photocatalyst efficiency for methylene blue degradation under simulated Solar illumination was assessed in an aqueous solution. Among the nanocomposites considered, TiO_2@rGO_8wt% was the most efficient, achieving 99.20 % MB photodegradation in 120 min. The same photocatalytic conditions were applied to natural water matrices (tap water, seawater, lake water, and river water) and using natural sunlight illumination to evaluate the influence of real conditions on the photocatalysis of prepared TiO_2@rGO nanocomposite. The photodegradation percentages obtained were efficient. Therefore, the results obtained for photocatalytic efficiency in the natural environment are promising, suggesting a great potential for application in green photocatalysis to remove methylene blue from wastewater in environments.

References

[1] M. Abd Elnaby Wafi, M.A. Ahmed, Hesham S. Abdel-Samad, Medien H.A.A., *Materials Science for Energy Technologies*, **5**, 217-231 (2022).

[2] J. F. Leal, S. M. A. Cruz, B. T. A. Almeida, V. I. Esteves, P. A. A. P. Marques, E. B.H. Santos, *Environmental Science: Water Research & Technology*, **6**, 1018-1027 (2020).

[3] I. Ali, M. Suhail, Z. A. Alothmanc, A. Alwarthanc, *RSC Advances*, **8**, 30125-30147 (2018)

[4] A. Mondal, A. Prabhakaran, S. Gupta, V. R. Subramanian, *ACS Omega*, **6**, 8734–8743 (2021)

O44. Polymorphous crystallization of amorphous films initiated by electron irradiation: classification and structural-morphological characteristics

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The passage of electrons through a film causes its Joule-Lenz heating (excitation of phonons) and can create radiation damage. In a certain mode of operation of the microscope, the electron beam that forms an image can initiate the crystallization of an object with an amorphous structure. In this case, film crystallization can be observed visually (“in situ” method). Based on in situ electron microscopic studies by video recording of phase transformations, following polymorphous crystallization modes in amorphous films have been identified based on the structural and morphological characteristics (Table 1):

Layer polymorphous crystallization (LPC) mode describes the nucleation and growth of a single-crystal layer in the zone of the electron-beam impact on amorphous film [1, 2]. In this case, relative length $\delta_0 = D_0/a_0$, where a_0 is a cell parameter of the growing crystal. D_0 is an average crystal size at a time $t = t_0$ (t_0 is a characteristic unit of time), after which the volume of the amorphous phase decreases by the factor of e = 2.718. For LPC mode δ_0 is about several thousand (3000-5000).

Island polymorphous crystallization (IPC) mode describes the nucleation and growth of a polycrystalline layer (Fig. 1). In this case, $\delta_0 = D_0/\Omega^{1/3}$, where Ω is the volume of the unit cell of a crystal. For IPC mode δ_0 is about several hundred (100-1100).

Dendrite polymorphous crystallization (DPC) mode describes the nucleation and growth of the dendrite in the amorphous layer [3]. In this case also $\delta_0 = D_0/\Omega^{1/3}$, where Ω is the volume of the unit cell of a crystal. For DPC mode $\delta_0 \sim 3000\text{-}4000$.

Table 1. Crystallization modes in amorphous films

Crystallization mode	Film	Deposition method	δ_0
LPC	Sb_2S_3	Thermal evaporation	4900
	Cr_2O_3	Laser evaporation	3100
	V_2O_3	Laser evaporation	4500
	Ta_2O_5	Laser evaporation	3600
IPC	ZrO_2	Ion-plasma evaporation	120
	ZrO_2	Laser evaporation	900
	Ta_2O_5	Laser evaporation	410
	V_2O_3	Laser evaporation	1020
	Yb_2O_2S	Electron beam evaporation	1030
DPC	HfO_2	Laser evaporation	3800

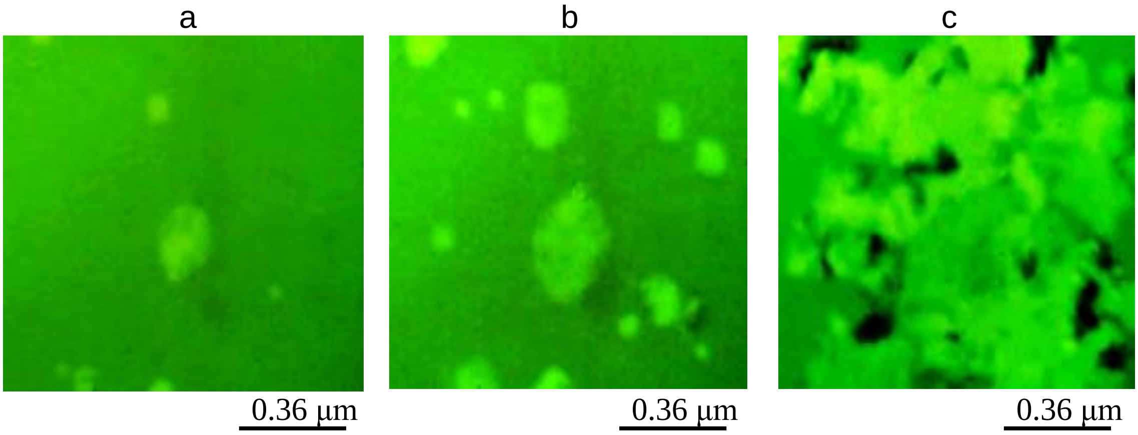

Fig. 1. IPC of amorphous film of Ta_2O_5. The micrographs correspond to the periods of time *t* that passed since the start of the recording: (a) *t* = 0.27 s; (b) *t* = 0.70 s; (c) *t* = 2.23 s.

References

[1] A. Bagmut, I. Bagmut, Nanomaterials Science & Engineering, **1**, 30 (2019).
[2] A. Bagmut, *Functional Materials,* **26,** 6 (2019).
[3] A. Bagmut, Problems of Atomic Science and Technology, **137(1)**, 64, (2022).

O45. Novel S-scheme based nanocomposite of MXene/V_2O_5 for photocatalytic degradation of Crystal Violet from Contaminated water

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In this study, a novel 2D/2D heterostructure of MXene and V_2O_5 was synthesized using facile hydrothermal approach for the efficient removal of crystal violet (CV), a textile dye from contaminated water. Here, the catalytic performance of pristine MXene was prominently boosted with the introduction of ball milled V_2O_5 as an electron generating agent. The degradation efficiency of synthesized heterostructure significantly enhanced from 57.3% to 92.8%, 41.3% to 76.5% and 7.1% to 58.6% as compared to pristine MXene at 10, 20 and 30 ppm concentrations of CV respectively, in 120 minutes. The effective degradation of pollutants is ascribed to the electron-transfer via S-scheme based mechanism and helps in reducing recombination rate of the photogenerated carriers, which could produce hydroxyl radicals $(OH^{\cdot})$ as the primary species for effectively degradation of the pollutants. The crystalline nature and analysis of functional groups was analyzed using X-ray diffraction (XRD) and Fourier Transform Infrared spectroscopy (FTIR). The optimized bandgap of synthesized samples was elucidated using Tauc's plot and proves favorable for the degradation of CV under NIR and visible region. The elemental composition, surface properties and formation of oxygen vacancies was analyzed using X-ray photoelectron spectroscopy (XPS). The study of surface charge and charge transfer resistance (R_{ct}) of synthesized samples was carried out using zeta potential and electron impedance spectroscopy (EIS) measurements. The results shows that the surface charge and R_{ct} of synthesized heterostructure supports for the degradation of CV dye as compared to pristine samples.

The enhanced values of carrier concentration in case of synthesized heterostructure and band-edge positions were analyzed using mott-Schottky (MSK) analysis. Moreover, to strong the findings of scavenger study electron paramagnetic resonance (EPR) study was also carried out and concluded that hydroxyl radicals $(OH^{\cdot})$ are the primary species in the mineralization of CV dye. The values of lande g-factor are also calculated using EPR plots which comes out to be 2.03 and 2.04 for $(O_2^{\cdot -})$ and $(OH^{\cdot})$ radicals, respectively and demonstrates the formation of free radicals during photocatalytic reactions. The reusability experiment confirms the stability of synthesized sample and provides a good shred for industrial applications of the synthesized samples in the treatment of wastewater and getting out the cleaner productions.

O46. A synergistic composite of rGO/MOF-5 for Electrochemical Energy Storage

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With the escalating population, development in the field of science and economy the energy demand is continuously increasing and so the use of fossil fuels. However, renewable energy sources based on solar energy, wind energy, tidal energy etc. are supplanting fossil fuels to scale down the greenhouse emissions. But their cons such as weather dependency, location specificity, high cost and low efficiency are pushing researchers towards advancement of energy storage devices like batteries, fuel cells, flywheels and supercapacitors (SCs). In contrast, due to their exceptional high-power densities, quick charge-discharge capabilities, prolonged cycle lifespans, and most significantly their focus on safety, (SCs) have attracted considerable attention. Biggest hurdle in the commercialization of supercapacitors is there low energy density. So search in on for some electrode electrolyte combination which can provide significantly high energy density. Due to ultrahigh porosity, exceptional surface area, robust structure and tunable properties Metal-Organic Frameworks (MOFs) are most emerging candidates for electrode materials in the present era. But the presence of organic linker is what made them less conducting and resists their use as electrode material. In our work we have synthesized Zinc metal ion based MOF-5 and it’s composite with reduced graphene oxide (rGO) using solvothermal method. All three samples were characterized using X-ray diffraction (XRD), Fourier transfrorm Infrared Spectroscopy (FTIR), Field Emission Scanning Electron Microscopy (FESEM), Braunner Emmett Teller (BET) for surface area measurement. The MOF-5/rGO composite shown a high surface area of 1148.2 m^2/g and a unique morphology in which MOF-5 particles were found resting on the rGO layers. Finally the samples were studied using Cyclic Voltammetry (CV), Galvanostatic Charge Discharge (GCD) and Electrochemical Impedence Specctroscopy (EIS). The composite material shown an exceptional specific capacitance of 1122.22 Fg^{-1} while a low solution resistance and charge transfer resistance.

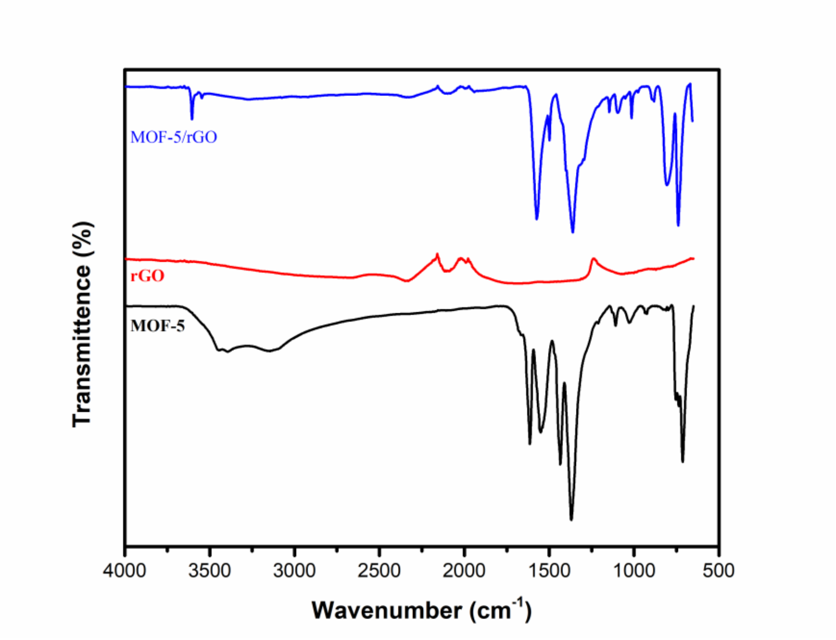

Fig. 1 Fourier Transform Infrared Spectroscopy Plot

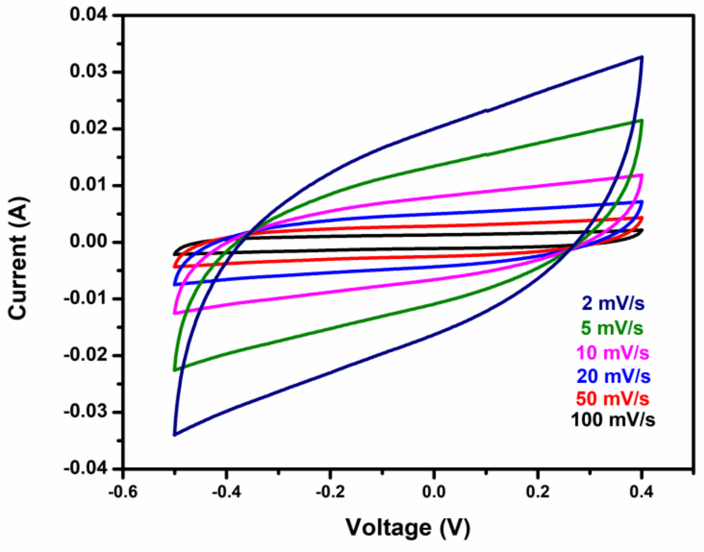

Fig. 2 Cyclic Voltammetry Curves of rGO/MOF-5

References

[1] Fan, W., Zhang, X., Kang, Z., Liu, X., & Sun, D, *Coord. Chem. Rev.*, *443*, 213968 (2021).

[2] Almáši, M., Zeleňák, V., Gyepes, R., Zauška, U., & Bourrelly, S., *RSC Adv.*, *10*(54), 32323–32334 (2020).

[3] Hao, M., Qiu, M., Yang, H., Hu, B., & Wang, X. (2021) *Sci. Total Environ. 760*, 143333

O47. Ex-Situ synthesis of Fe_2O_3-TiO_2 nanocomposites for photocatalytic applications

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Titanium oxide and Fe2O3 were opted nanocomposite because of their optical properties, Band gap which is 3.27ev and 2.2 eV respectively, thermal stability and photo catalytic activity. Safranin and Rhodamine6G dye are degraded at higher rate using coupled semiconductor Fe2O3/TiO2 than individual Fe2O3 and TiO2. The proposed method can also be used for synthesizing other semiconductor TiO2 containing nanoparticle.

O48. Synthesis of organic-inorganic semiconductor photocatalysts and their composites for environmental remediation

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The investigation of diverse materials, including carbon and metal oxide-based semiconductors, leading to the successful synthesis of novel photocatalysts. Key highlights include the controlled fabrication of nano-sized two and three-dimensional ZnO structures, demonstrating exceptional photocatalytic performance in the degradation of methylene blue. Additionally, the study pioneers the synthesis of pentacenequinone (PQ) through a green and innovative solid-state method, showcasing its viability as a visible light-active photocatalyst. The integration of PQ with ZnO yields a remarkable nanocomposite with an impressive degradation efficiency. This work not only contributes to the dominion of visible-light-driven photocatalysts but also opens new avenues for future research in the realm of environmental purification. The findings the way for innovative and sustainable solutions, propelling the boundaries of photocatalysis and materials science to address contemporary challenges in water pollution and beyond.

O49. Nanostructures and applications

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Abstract:

Nanotechnology is an interdisciplinary field that studies materials and structures of billionths in size and their uses. Nanomaterials are the cornerstones of nanotechnology and have unique optical, magnetic and electrical properties. What makes nanotechnology so interesting is that materials behave differently in this dimension than in the macro world. The power/weight ratio, conductivity, optical and magnetic properties change significantly as you move from the macro dimension to the nano dimension. The aim of this study is to critically examine nanostructures and their applications. Within nanostructures, nanomachines, nanorobots as well as nanosensors have been explained and critically discussed. Then, nanostructure applications in the automotive industry, energy, defense and environmental fields are systematically explained, and finally, a future-oriented perspective on nanostructure is given to motivate young generations to research and to point out the deficiencies in the related field of study.

1. Introduction

About arrangement, nanomaterials have tremendously trivial dimensions and as a minimum one dimension is 100 nm or smaller. Nanomaterials can be nanoscale in one, two or three dimensions. They can be found in single, fused, clustered or clustered forms with tubular, spherical and uneven forms [1]. Communal kinds of nanomaterials comprise fullerenes, nanotubes and quantum dots. Nanomaterials have uses in the area of Nanotechnology and show dissimilar physical chemical properties from normal chemicals such as Silver Nano, Fullerene and Silica) [2].

Perspectives on nanostructures essential to encompass the insights and boundaries of numerous systematic disciplines. It has been stated that the benefit of nanostructures will be its application in catalysis, but the chemist is also investigating nanoscale materials and must ensure that quantum detention effects are displayed. Nanometer-sized materials are best articulated in optical or electronic technology, where the nanostructure can be insulated from the molecules encountering, thus avoiding any chemistry risks [3]. The aim of this study is to critically examine nanostructures and their applications. Within nanostructures, nanomachines, nanorobots as well as nanosensors have been explained and critically discussed. Then, nanostructure applications in the automotive industry, energy, defense and environmental fields are systematically explained, and finally, a future-oriented perspective on nanostructure is given to motivate young generations to research and to point out the deficiencies in the related field of study.

2. Nanostructures

Nanostructures are synthetic and are structures ranging from 1 nm to 100 nm. Nanostructures can be designed according to a wide variety of physical properties such as nanosurfaces and cylindrical nanotubes.

2.1 Nano-machines

Nanomachines, the smallest of which are the size of a virus, are much smaller than a human cell and are usually expressed in micrometres. As nanorobots emerged, researchers turned to natural biological technology for motivation because most robotic construction techniques at this scale would be impossible. They are not made of metals that come to mind when robots are mentioned. Alternatively, nanomachines are made of DNA or other biological materials that seamlessly interact with the biological environment in certain ways to achieve specific results.

2.2 Nano-robots

Nanorobotics is the engineering discipline that includes the design and construction of nanorobots. It covers the construction of devices, tools and systems with nanoscale components or molecular components in 0.1-10 micron sizes.

2.3 Nano-sensors

The nanosensor transforms the data and information obtained from the atomic scale and nanoparticles into analyzable macro scales. Its biggest advantage is that it can work in small places that macro- and micro-sensors cannot reach; require less power in their operation; higher precision and adaptability for specific purposes.

3. Applications

Nanostructures can be applied in many places. In this part, few of them including automotive industry, energy, defense as well as environmental applications.

4. Future perspective

A rapidly changing “Nano World” with developments, innovations and new discoveries in nanosciences and nanotechnology may take shape in our future. It is calculated that nanotechnologies, together with their key roles and rapidly combining with information-communication, biology and cognitive sciences, will create vast innovation opportunities in all other science and technology fields.

5. Conclusion

Nanotechnology uses the results from the emergence of new properties of matter at the nanoscale. At the nano level, the chemical and physical properties of matter differ considerably. Nanosensors, Nanomachines and nanorobots are important systems used in nanostructures.

References

[1] F. Trotta and A. Mele (Ed.), “*Nanomaterials: Classification and Properties*”, in Nanosponges: Synthesis and Applications: First Edition, Wiley, London, (2019).
[2] Fehim Findik, *Periodicals of Engineering and Natural Sciences*, **Vol. 9**, No. 3, pp.62-75 (2021).
[3] A.S Edelstein, R.C Cammaratra, *Nanomaterials: Synthesis, Properties and Applications*, Second Edition-Taylor & Francis (1998).

Poster presentations

P1. Mechanical Characterization and Potential Device Fabrication of p-Toluenesulfonate Based Compounds for Nonlinear Optical Applications

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p-Toluenesulfonate based compounds have emerged as vital materials in the field of photonics and optoelectronics, owing to their remarkable ability to generate, manipulate, and control light at the molecular level. These organic nonlinear optical (NLO) materials exhibit nonlinear responses, enabling a wide range of applications including frequency conversion, optical switching, and signal processing. The exceptional optical properties of these materials emerge from their possession of a highly delocalized electron cloud. The interaction between photons and this electron cloud gives rise to various phenomena, such as second harmonic generation (SHG), electro-optic (EO) effect, and two-photon absorption (TPA). To explore the potential of p-toluenesulfonate based compounds, high-quality NLO crystals were grown using the solution growth technique (SEST). This study focuses on three specific compounds: L-alaninium p-toluenesulfonate (LAPT), L-threonine p-toluenesulfonate monohydrate (LTPTM), and nicotinium p-toluenesulfonate monohydrate (NPT). In this work, the mechanical properties of these crystals were investigated using the nanoindentation characterization technique. The objective was to assess their mechanical strength and evaluate their suitability for device fabrication in nonlinear optical applications. Results indicate that LAPT possesses the highest hardness among the studied compounds, followed by LTPTM and NPT. These materials hold great promise for the development of efficient devices in the field of nonlinear optics.

P2. Electrochemical behavior of dopamine on the surface of electrodes modified with manganese ferrite nanoparticles

Lizz Gabi Luza Mamani[1], Edilson Valmir Benvenutti[1], Tania Maria Haas Costa[1], Eliana Weber de Manezes[1], Sabrina Nicolodi[2], Leliz Ticona Arenas[1]

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Recently, metal oxide nanoparticles (NPs) have contributed to the development of more sensitive and efficient electrochemical sensors with better selectivity [1]. Electrodes modified with manganese ferrite ($MnFe_2O_4$) will increase electroactive area and provide high transfer kinetics, improving the properties of the electrode [2]. In this context, $MnFe_2O_4$ NPs were obtained with different properties, and were made carbon paste electrodes (CPE), and it was evaluated the response of dopamine (DA).

The NPs were obtained by coprecipitation and hydrothermal method, using $MnSO_4$ and $FeCl_3$ (1:2) as precursors at 140°C for 24h, NPs were also prepared under similar conditions using β-cyclodextrin as stabilizing agent, this sample was named as CD-$MnFe_2O_4$.The samples show magnetic behavior, XRD analysis indicated the presence of monophasic manganese ferrite with a crystallite size of 20nm for $MnFe_2O_4$ and 5nm for CD-$MnFe_2O_4$. The NPs possessed high BET area values of $170m^2g^{-1}$ and $240m^2g^{-1}$ for $MnFe_2O_4$ and CD-$MnFe_2O_4$ respectively, the molability of the NPs surfaces was measured using the contact angle technique, being 110º for $MnFe_2O_4$ and 53° for CD-$MnFe_2O_4$ characterizing hydrophobic and hydrophilic surfaces respectively.

Differential pulse voltammetry measurements of the modified CPE in the presence of DA indicated that the oxidation was at 0.16V for CPE-$MnFe_2O_4$ and at -0.16V for CPE-CD-$MnFe_2O_4$. Analysis of interferents showed that CPE CD-$MnFe_2O_4$ is more selective for DA, because no interference from analytes such as ascorbic acid and uric acid, was observed, meanwhile, in the CPE-$MnFe_2O_4$ was observed that these analytes interfere a dopamine response. The electrodes showed a good linear range, low limited the detection of DA and good sensitivities.

References

[1] S.R. Sabale. Mater. Today. Proc.33,139-146 (2020).,
[2] B.M. Asiabar, M.A. Karimi, et al. Microchem. J., 161 (2021)

P3. Oxidation of 1-hexene using supported nano-catalysts under solvent-free conditions

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Empty Quarter research Unit, Department of Chemistry, College of science and art in Sharurah, Najran University, Saudi Arabia
** Presenter's Email: kaade_77@hotmail.com. Phone: 00966551519221*

The present work employs supported ruthenium nanoparticles alongside catalytic quantities of the radical initiator, which are proven to be capable of 1-hexene oxidation with green conditions, in the absence of solvent, with air as the main oxidant and without sacrificial reductant. The paper examines the effects of a range of radical initiators and how the products are distributed over time. Furthermore, this work addresses the reaction pathways to the epoxides and other products. Catalyst activity can be markedly improved by adopting a sol-immobilization technique to synthesise the catalysts.

P4. Carbon dots as a reinforcement agent in recycled HDPE

Raul Simões[1,2,*], Gil Gonçalves[1], Teresa Monteiro[2] and Victor Neto[1]

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The intense use of plastic, where large fraction is designed to be discarded almost immediately, with only 9% recycled, being the remaining discharged in landfills and, ultimately, in the environment. Additionally, global production of plastics is expected to be duplicated in the next 20 years. [1] With the technology progress and rising demand for sustainable solutions, especially for polymeric parts with specific properties, it is important to develop new materials and recycling strategies. Thus, one solution is nanoparticles incorporation, such as carbon-based nanoparticles, to create brand new nanocomposites with improved mechanical properties. In this study, carbon dots (CDs) have been chosen to be incorporated into the polymer HDPE (high density polyethylene) using three different concentrations, to evaluate its influence in the nanocomposite's mechanical properties. The next step was to further recycle the nanocomposites to evaluate how the presence of CDs affect parameters such as tensile strength, yield strain, hardness modulus and elastic modulus. Those mechanical properties were defined through nanoindentation and mechanical testing to study their suitability for further usage. The results showed improved tensile strength and yield strain for a filler concentration of 0.5% after being recycled more than once. This a good indicator for improved mechanical properties in HDPE:CDs nanocomposites.

References

[1] J. Pinto Da Costa, T. Rocha-santos, and A. C. Duarte, “The environmental impacts of plastics and micro-plastics use, waste and pollution: EU and national measures - Requested by the PETI committee. European Union - PE 658.279,” no. October, pp. 1–72, 2020.

P5. Effect of Cobalt doping on structural optical and electrical properties of sputtered nickel oxide thin films

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Cobalt doped Nickel oxide thin films were synthesized by the reactive radio frequency (RF) sputtering glass substrates. The influence of the ratio Co/Ni on the structural, optical and electrical NiO thin films was investigated. The X-ray diffraction (XRD) analyses show that there is one peak privileged to (200) plane with cubic structure. The crystallite size and crystallinity decreases versus the ratio Co/Ni. The dislocation and microstrain increase but d_{hkl} and lattice parameter decrease. Scanning electron microscopy (SEM) shows a smooth surface with columnar structure, but the doping change the form of grains. Transmittance and band-gap were carried out by UV-Vis-IR spectrophotometer, are both obtained to be decreased with doping ratio. The electrical properties were carried out by Hall effect measurement, the lowest resistivity was obtained 0.057 for the Co/Ni ratio 1.6 %

P6. Structural, Optical and Electrical Properties of Ternary Composites OF $BiFeO_3$-Graphene- $KNbO_3$

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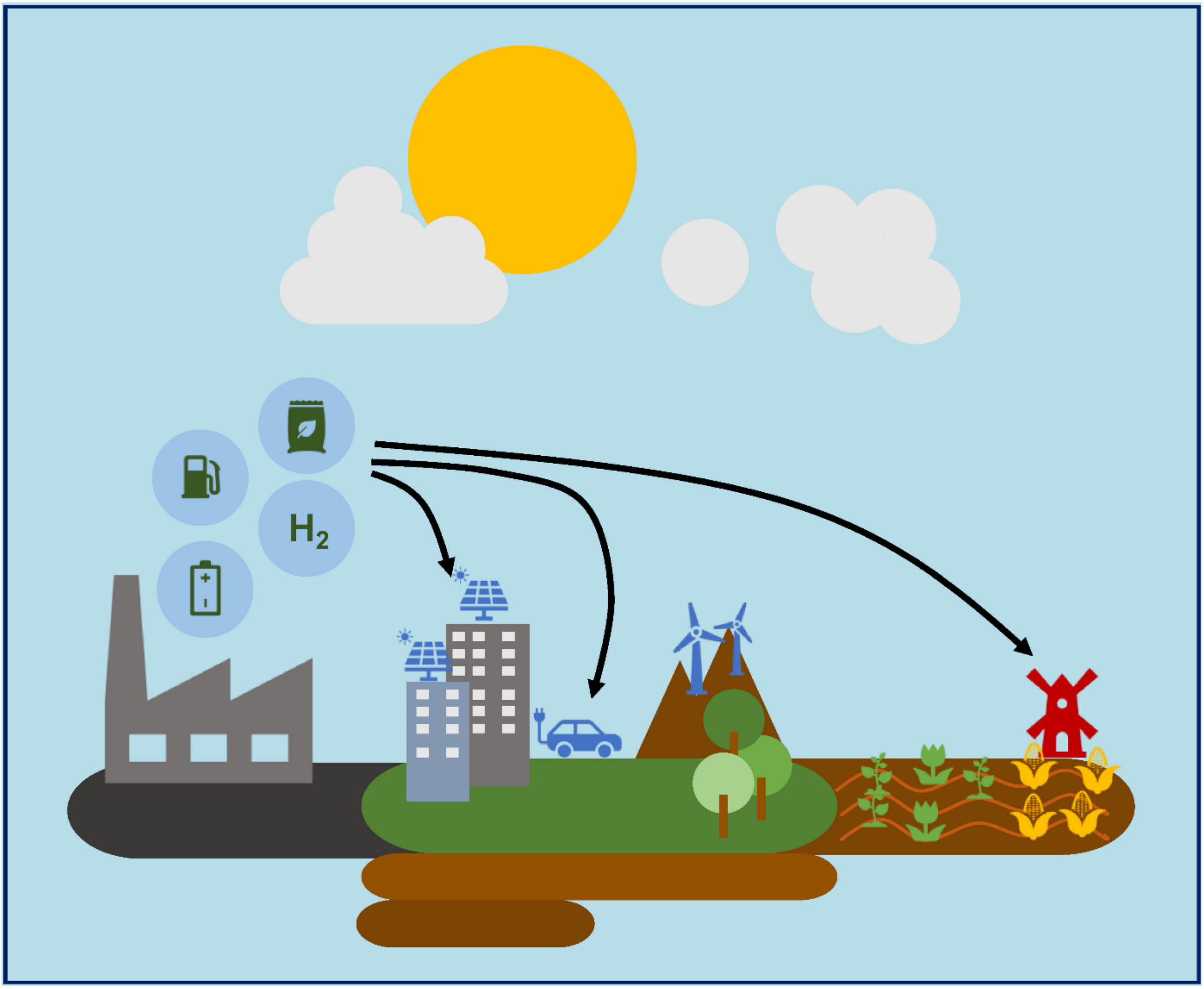
Perovskite material have gained more attention due to its physical characteristics and potential applications. The combination of two perovskite material helps to improve the electrical properties. In addition, to enhance the transfer of photo induced charge carries between two perovskite admixture with help of graphene due its high electron conductivity. So, herein prepared a new type of ternary nanocomposites of $BiFeO_3$(BFO)-Graphene(Gr)-$KNbO_3$(KN) by the solution method. Study the effect of Gr content (0.025, 0.050, 0.075, 0.1) on BFO-KN composite are in details. The synthesized ternary compounds have been characterized by various technique like powder X-ray diffraction, Raman spectroscopy is used to study phase formation and its related vibrational bands. Field Emission-Scanning Electron Microscopy with EDX (Energy dispersive X ray spectroscopy) analysis use to see the morphological changes and corresponding composition. UV-Vis-NIR spectroscopy is used to obtain various electronics transitions and its changes in the density of states, in addition the direct and indirect band gap changes with respect to Gr content also derivate. The ternary composites are aided to tune the band gap value which may use many optical applications. The sticking changes in the bulk dielectric and ac- conductivity clearly indicates the effect of the conducting material dispersed in an admixture of a perovskites.

References

[1] Sabeen Fatima and Syed Rizwan, ACS Omega, **8**, 3736 (2023).
[2] S. Raja, K. Arjunan, R. Mahalakshmi, B. Noorul Ayin and R. Ramesh Babu, *AIP Conf. Proc.* **2265**, 030577 (2020).
[3] Pan Zhang, Yanqing Shen, Wenjing Wu, Jun Li and Zhongxiang Zhou, Appl. Surf. Sci. **434,** 932 (2018).

Workshop 1

1st International Workshop on “Modern Trends in Energy Research”
20 November 2023, Aveiro, Portugal



Topics:

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

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Program committee:
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Workshop Website:
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1st International workshop on “Modern Trends in Energy Research”
20 November 2023, Aveiro, Portugal

List of talks and the presentation schedule

Date: 20/11/2023

Session 1 – 9.30 h to 11.30 h

Session chair: Duncan Paul Fagg

1	***Plenary Lecture*** **Gunnar Suchaneck: 9.30 to 10 h** *TU Dresden, Solid-State Electronics Laboratory, 01062 Dresden, Germany.* Title: **Solid oxide fuel cells based on nonstoichiometric strontium ferromolybdate electrodes**
2	**W1-O1** **Allan J. M. Araújo: 10.00 to 10.20 h** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.* Title: **Transition metal carbides as potential anode components for Proton Ceramic Fuel Cells (PCFCs)**
3	**W1-O2** **Alfredo S. B. Luemba: 10.20 to to 10.35 h** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.* Title: **Synthesis of carbon and sulfur-resistant electrolytes for proton ceramic membrane reactors**
4	**W1-O3** **E. Durana: 10.35 to 10.50 h** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.* Title: **Reversible electrodialysis: a salinity gradient power source**
5	**W1-O4** **Ihsan Çaha: 10.50 to 11.05 h** *International Iberian Nanotechnology Laboratory, Avenida Mestre José Veiga s/n, 4715-330 Braga, Portugal.* Title: **Chemical bath deposition of $Zn_{1-x}Sn_xO_y$ thin films and their application as buffer layers for Cd-free $Cu(In, Ga)Se_2$ solar cells**
6	**W1-O5** **Catarina de Lemos: 11.05 to 11.20 h** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.* Title: **Study of rGO-MIL101(Cr) as the anode of a half-cell**

11.20 to 11.30: Interval

Session 2 – 11.30 h to 13.00 h Session chair: Gil Gonçalves

7	**W1-O6** **Francisco J. A. Loureiro: 11.30 to 11.50 h** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.* **Title: TiO_2/MgH_2-based anodes for lithium-ion batteries**
8	**W1-O7** **Thayse R. Silva: 11.50 to 12.05 h** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.* Title: **Compositional optimization of $MnCo_2O_4$@rGO electrocatalysts for oxygen evolution reaction**
9	**W1-O8** **Laura I. V. Holz: 12.05 to 12.25 h** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.* Title: **Exploring Vanadium (Oxy)nitride as a Promising Anode Material for Ammonia Solid Oxide Fuel Cells**
10	**W1-O9** **Paula Rosendo Santos: 12.25 to 12.45** *Universidad San Pablo-CEU, Facultad de Farmacia, Departamento de Química y Bioquímica, Urbanización Montepríncipe, Boadilla del Monte, E-28668, Madrid, Spain.* Title: **Optimization of the electrochemical performance of Nd1/3Sr2/3CoO3−δ cathode for solid oxide fuel cells via spray-pyrolysis deposition and decoration with Ag nanoparticles**
11	**W1-O10** **D. Pukazhselvan: 12.45 to 13.00 h** *TEMA - Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.* Title: **Comments on the suitable hydrogen storage materials for vehicular applications**

W1-PL1. Solid oxide fuel cells based on nonstoichiometric strontium ferromolybdate electrodes

Gunnar Suchaneck[*], Evgenii Artiukh

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This contribution is devoted to the application of $Sr_2FeMoO_{6-\delta}$ (SFM) and $Sr_2Fe_{1.5}Mo_{0.5}O_{6-\delta}$ (SF$_{1.5}$M) in $La_{1-x}Sr_xGa_{1-y}Mg_yO_{3-\delta}$ (LSGM)-based solid oxide fuel cells (SOFCs). We consider the most relevant physical properties (crystal structure, thermodynamic stability, iron and molybdenum valence states, oxygen vacancy formation and oxygen non-stoichiometry, electrical conductivity), A- and B-site ion substitution in such $AB'B''O_6$ double perovskites, and the performance of $Sr_2Fe_{1+x}Mo_{1-x}O_{6-\delta}$ (SF$_{1+x}$M) SOFCs (polarization resistance, operation with hydrogen, operation with hydrocarbons and methanol). SF$_{1+x}$M materials are excellent catalysts in hydrocarbon oxidation and can prevent carbon deposition due to the ability to exchange lattice oxygen with the gaseous phase. Moreover, they are sulfur tolerant. This opens the way to direct hydrocarbon fueled SOFCs, eliminating the need for external fuel reforming and sulfur removal components. Such SOFCs can be greatly simplified and operate with much higher overall efficiency thus contributing to the solution of the lack of energy problem in our modern world [1]. Summarizing crystal structure, thermodynamic stability, Fe and Mo valence state, and oxygen vacancy formation generation energy, SF$_{1.5}$M is a compromise that provides a cubic crystal structure, generates an electronic structure as well as oxygen vacancies that promote suitable electrical transport properties and catalytic activity in oxidizing and reducing atmospheres. The electrocatalytic properties of SF$_{1.5}$M may be further improved by partial substitution of A-site and B-site ions. The partial substitution of A and/or B site elements is an effective way to improve the performance perovskite-type materials. The additional introduction of alkali earth metal elements on the A-site and transition-metal elements on the B-site affects the cation valence and oxygen-vacancy concentration, and thus improves the electronic or ionic conductivity of the material as well as its catalytic properties.

This research was funded by the European Union within the scope of the project H2020-MSCA-RISE-2017-778308–SPINMULTIFILM.

References

[1] G. Suchaneck, E. Artiukh, *Inorganics*, **10**, 230 (28pp) (2022).

W1-O1.Transition metal carbides as potential anode components for Proton Ceramic Fuel Cells (PCFCs)

<u>Allan J. M. Araújo</u>[1,2]*, Sergey M. Mikhalev[1,2],
Duncan P. Fagg[2,3], Francisco J. A. Loureiro[1,2]

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Proton ceramic fuel cells (PCFCs) provide an environmentally friendly solution for generating electricity and heat through the electrochemical conversion of hydrogen or hydrocarbon-based fuels. Regarding cell configuration, it is well-established that anode-supported cells demonstrate superior electrochemical performance when compared to cells supported by cathodes or electrolytes [1]. Nickel-based cermets are usually employed as anodes due to their exceptional catalytic properties in fuel oxidation and effective current collection [2]. However, nickel faces several functional limitations when fuelled with hydrocarbons, such as carbon surface deposition. This issue significantly impacts the electrochemical performance, leading to degradation over the course of their operation [2]. In this preliminary study, transition metal carbides (TMCs, namely Mo_2C, NbC, WC and ZrC) are investigated for application as potential anode materials. Excellent phase stability is observed in a methane (CH_4) atmosphere at 900 °C for 24 h. In addition, there is no evidence of any chemical interreaction between the carbides and the electrolyte material, $Ba_{0.852}Zr_{0.148}O_{3-\delta}$. The coefficient of thermal expansion, determined through dilatometry, falls within the range of 7 x 10^{-6} to 8 x 10^{-6} °C^{-1} from 100 °C to 700 °C, which is close to that typically reported for PCFC electrolytes, *i.e.*, 9 x 10^{-6} to 13 x 10^{-6} °C^{-1} [3]. Lastly, electrical properties assessed via the 4-probe method reveal a metal-like behaviour, with the electrical conductivity increasing with decreasing temperature. These findings demonstrate that the proposed TMCs represent a promising new material' category of anodes suitable for utilisation in PCFCs, especially in carbonaceous environments.

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References

[1] M. E. Chelmehsara and J. Mahmoudimehr, *Int. J. Hydrogen Energy*, **43**, 15521 (2018).
[2] F. J. A. Loureiro, G. S. Souza, V. C. D. Graça, A. J. M. Araújo, J. P. F. Grilo, D. A. Macedo, and D. P. Fagg, *J. Power Sources*, **438**, 227041 (2019).
[3] Z. Li, M. Peng, Y. Zhao, J. Li, Y. Sun, *Nanoscale*, **13**, 20299 (2021).

W1-O2. Synthesis of carbon and sulfur-resistant electrolytes for proton ceramic membrane reactors

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The dependence on fossil fuels has been one of the leading causes of climate change, driving up the earth´s temperature and fundamentally changing the world around us, causing environmental pollution on the planet. However, since 2000, global energy consumption has grown exponentially due to social and economic development worldwide. For this reason, the European Union (EU) leaders signed an agreement to mitigate the greenhouse gas effect by 2050, guaranteeing the supply of safe, clean, and affordable energy in Europe [1,2].

According to the International Energy Agency (IEA), biogas can be critical in this goal, as these gases can transform the global energy system. Along this path, biogas can be converted into H_2-rich gas using the reforming process to generate helpful fuel or raw material for chemical production [3].

Following these aims, the current study proposes an electrochemical configuration to form green syngas (a mixture of CO and H_2) from a biogas precursor, by direct electrochemical pumping across a proton-conducting ceramic-oxide membrane [4]. In this regard, perovskite proton-conducting ceramics of the ABO_3 structure with the specific composition of $BaZr_{1-x}Y_xO_{3-d}$ (x = 0, 0.15, and 0.2) family were synthesized using different processing methods: the acetate combustion route and the mechanosynthesis.

References

[1] Polcyn J, Us Y, Lyulyov O, Pimonenko T, Kwilinski A., *Energies*, 2022, 15, 1–27. (https://doi.org/10.3390/en15010108).

[2] European Parliament. Fact Sheets on the European Union: Renewable energy 2021. (https://www.europarl.europa.eu/factsheets/en/sheet/70/renewable-energy (accessed on September 2023).

[3] International Energy Agency. Global Energy Review: CO_2 Emissions in 2021 (https://iea.blob.core.windows.net/assets/c3086240-732b-4f6a-89d7-db01be018f5e/GlobalEnergyReviewCO2Emissionsin2021.pdf (accessed on September 2023).

[4] Francisco J. A. Loureiro, Domingo Pérez-Coll, Vanessa C. D. Graça, and Duncan P. Fagg, *J.* Mater. Chem. A, 2019, 7, 18135-18142 (https://doi.org/10.1039/C9TA04584H).

Acknowledgments

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W1-O3. Reversible electrodialysis: a salinity gradient power source

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The energy demand in the last decades has been increasing globally, mainly caused by population growth and rising living standards in emerging countries. Modern society still relies heavily on limited and pollutant fossil fuels. Greenhouse gas emissions and global warming impacts are forcing the search for alternative clean and green energy resources [1].

The Salinity Gradient Power (SGP) is a clean and renewable energy source based on the salinity difference between sea and river water. The potential energy from SGP, using the salinity difference between seawater and freshwater flows, is comparable to the potential energy associated with a 280-meter-high dam. Theoretically, it would be possible to extract 0.8 kilowatts per cubic meter of fresh water. The combined river water running to the sea in the world's estuaries has been predicted to harness 980 GW of electric power. An additional 18 GW could be obtained by using wastewater released in the ocean [1].

Reverse electrodialysis (RED) is a sustainable technology that uses SGP to produce electricity by mixing different salinity water feeds. RED non-intermittent electrochemical process employs ion-exchange membranes (IEMs) for *Donnan* potential generation. The device open circuit voltage (OCV) results from the voltage across each IEM stacked. The electrochemical potential at the electrodes is converted to electricity by a reversible redox reaction [2]. RED can increase energy efficiency using water effluent from industrial processes [3].

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References

[1] B. E. Logan and M. Elimelech, *Nature*, **488**, 313 (2012).
[2] R. A. Tufa et al., *Applied Energy*, **225,** 290 (2018).
[3] A. Nazif et al., *Journal of Water Process Engineering,* **47**, 102706 (2022).

W1-O4. Chemical bath deposition of $Zn_{1-x}Sn_xO_y$ thin films and their application as buffer layers for Cd-free Cu(In, Ga)Se_2 solar cells

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Cu(In, Ga)Se_2 (CIGSe) thin-film solar cells have gained significant attention as a promising solution for the current energy challenge due to their low cost and potential for flexible, tandem, or semi-transparent applications. These cells have a record power conversion efficiency (PCE) of 23.4% [1-4]. However, the conventional use of toxic CdS buffer layers in these devices poses environmental and health concerns. In this study, we explored the feasibility of using $Zn_{1-x}Sn_xO_y$ (ZTO) thin films as Cd-free buffer layers for CIGSe solar cells. ZTO has emerged as a promising alternative buffer material due to its non-toxicity, fast light responsivity, and tunable wide band gap. Previous studies have only deposited ZTO buffer layers by atomic layer deposition, which is hardly scalable, time-consuming, and expensive.

To overcome this challenge, we synthesized ZTO films by chemical bath deposition (CBD), which is a cheap, easy-scalable, low-temperature technique. The resulting ZTO films had a flatter morphology than reference ZnO, and our findings also revealed a non-trivial increase in the band gap upon increasing Sn concentration. We achieved similar device performance to CdS buffer layers (with an average efficiency of (11 ± 2)%), with a maximum efficiency of 10.4%, and an average of (9 ± 2)% when using a ZTO buffer layer with a concentration of 20% [Sn]/([Sn]+[Zn]) in the chemical bath [5].

References

[1] A.1T. D. Lee, A. U. Ebong, Renewable Sustainable Energy Rev. 2017, 70, 1286.
[2] Ramanujam, D. M. Bishop, T. K. Todorov, O. Gunawan, J. Rath, R. Nekovei, E. Artegiani, A. Romeo, Prog. Mater. Sci. 2020, 110, 100619.
[3] R. E. Agbenyeke, S. Song, B. K. Park, G. H. Kim, J. H. Yun, T.-M. Chung, C. G. Kim, J. H. Han, Prog. Photovoltaics Res. Appl. 2018, 26, 745.
[4] R. Fonoll-Rubio, M. Placidi, T. Hoelscher, A. Thomere, Z. J. Li-Kao, M. Guc, V. Izquierdo-Roca, R. Scheer, A. Pérez-Rodríguez, Sol. RRL 2022, 6, 2101071.
[5] Diego A. Garzón, Christian Rossi, Ishwor Khatri, Francesco Soggia, Ihsan Çaha, Francis Leonard Deepak, Diego Colombara, Sascha Sadewasser, Sol. RRL 2023, 7, 2300173

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W1-O5. Study of rGO-MIL101(Cr) as the anode of a half-cell

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Abstract: Advanced electrode materials with an improved specific capacity and performance are currently in the scope for the development of Li-ion batteries (LIBs). Researching the performance as anode materials for half-cells comprises several evaluations and specifically, rGO-MIL101(Cr) was used as anode in an assembled Li-ion half-cell in this study. MIL-101(Cr), a precursor metal-organic framework (MOF) constitutes one of the most attractive materials for energy storage, although it has a low-conductivity nature. To overcome it, nanoparticles have been incorporated through NH_3 treatment to form rGO, a procedure reported by Sandoval et al [1, 2]. The novel as-prepared material was inspected using XRD and used as an anode in an assembled half-cell. In a freshly made battery, Impedance was measured and electrochemical impedance spectroscopy (EIS) to identify the reaction mechanisms. Cyclic voltammetry (CV) profile and their polarization curves for the electrooxidation were analyzed. The outcome of electrochemical studies are very encouraging, proving the material chosen has characteristics to be used in energy storage.

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References

[1] Sandoval, S., Kumar, N., Sundaresan, A., Rao, C. N. R., Fuertes, A., & Tobias, G. (2014). *Chemistry–A European Journal*, *20*(38), 11999-12003..
[2] Sandoval, S., Kumar, N., Oro-Solé, J., Sundaresan, A., Rao, C. N., Fuertes, A., & Tobias, G. (2016). *Carbon*, *96*, 594-602.

W1-O6. TiO_2/MgH_2-based anodes for lithium-ion batteries

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Lithium-ion batteries (LIBs) have emerged as the primary choice for portable devices and electric vehicles due to their long-life cycle, high energy density, reasonable production cost, and device design flexibility [1]. This work explores the electrochemical performance of a 10 wt% MgH_2-added titania anode for Li-ion half-cell batteries. We used a distribution function of relaxation times (DFRT) analysis for quantifying the sources of polarisation losses from the impedance data. We observed a notable increase in both ohmic and polarisation resistance terms for the TiO_2+10 wt% MgH_2 compared to the standard titania anode. Moreover, the modified electrode shows a higher lithium diffusion coefficient than pure TiO_2, with capacity retention reaching 300 mA h g^{-1} at 0.1C. After charge/discharge cycles, the formation of a Li-incorporated crystalline structure is revealed in the case of a neat TiO_2 anode. Simultaneously, considerable changes in the crystallinity and microstructure are shown upon lithium insertion for MgH_2 added titania. Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM) studies suggest that a significant morphological evolution occurs upon operation.

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References

[1] S. Goriparti, E. Miele, F. De Angelis, E. Di Fabrizio, R. Proietti Zaccaria, C. Capiglia, *J. Power Sources*, **257**, 421–443 (2014).

W1-O7. Compositional optimization of $MnCo_2O_4$@rGO electrocatalysts for oxygen evolution reaction

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Improving the efficiency of electrocatalysts used as anodes in the oxygen evolution reaction (OER) represents a fundamental strategy in advancing the water splitting process, as it constitutes the stage that limits the overall reaction rate [1]. Spinel-type cobaltites, with their multiple oxidation states, are attractive materials in various technological domains, particularly in the field of water electrolysis [2]. In this work, the electrocatalytic properties of a series of $MnCo_2O_4$@reduced graphene oxide ($MnCo_2O_4$@rGO) composite electrodes are studied as a function of composition in alkaline medium (1 M KOH, *p*H = 13.8). The composite with 20 wt.% GO exhibits the lowest overpotential, 281 mV *vs.* RHE at 40 mA cm^{-2}. Electrochemical impedance spectroscopy (EIS) results recorded during the OER regime demonstrated a decrease in the resistive component associated with surface intermediates upon the addition of rGO. This phenomenon can be attributed to the heightened Faradaic reaction, which is facilitated by enhanced electronic conduction. Furthermore, excellent electrochemical stability was achieved within the current density range of 10 mA cm^{-2} to 60 mA cm^{-2} over 120h.

References

[1] J.S. Kim, B. Kim, H. Kim, K. Kang, Adv. Energy Mater., 8, 1702774 (2018).
[2] I. Nikolov, R. Darkaoui, E. Zhecheva, R. Stoyanova, N. Dimitrov, T. Vitanov. J. Electroanal. Chem., 429, 157-168 (1997).

W1-O8. Exploring Vanadium (Oxy)nitride as a Promising Anode Material for Ammonia Solid Oxide Fuel Cells

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Ammonia (NH_3) stands out as a promising energy carrier for utilization as fuel in solid oxide fuel cells (SOFCs). However, a persistent challenge exists in the quest for alternative anode materials that can enhance both the durability and performance of SOFC components [1-2]. To address this challenge, we have developed a novel composite anode material consisting of vanadium oxynitride (VON) as the electronic conducting phase and 8YSZ as the oxygen ion conducting phase. This anode material was fully characterized using various techniques, including X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), thermogravimetric analysis (TGA), and Electrochemical Impedance Spectroscopy (EIS).

Our findings revealed a good chemical compatibility between the two phases, particularly under reducing conditions (10%H_2 - 90%N_2) at elevated temperature (1150 °C). TGA analysis demonstrated the thermal stability of VON under these reducing conditions, exhibiting minimal mass changes due to minor variations in the N/O ratio. When subjected to an ammonia-rich environment, the electrode mechanism was evaluated using EIS over a temperature range of 650-800 °C, showing similarities to typical Ni-based cermets operating in a hydrogen atmosphere. Notably, we observed that the polarization resistance (R_p) was highly influenced by the ammonia flow rate, increasing as the flow rate increases, primarily due to diffusion and gas conversion limitations. The present work explores for the first time the use of VON as an anode for NH_3-SOFCs, thus offering valuable insights into the potential of this innovative material for enhancing the performance of ammonia-based solid oxide fuel cells.

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.

W1-O9. Optimization of the electrochemical performance of $Nd_{1/3}Sr_{2/3}CoO_{3-\delta}$ cathode for solid oxide fuel cells via spray-pyrolysis deposition and decoration with Ag nanoparticles

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Single-step synthesis and deposition of composite solid oxide fuel cell cathodes of composition $Nd_{1/3}Sr_{2/3}CoO_{3-\delta}$: $Ce_{0.9}Gd_{0.1}O_{1.95}$ (NSC:CGO; 70:30 w:w) with and without the addition of Ag nanoparticles (Ag NPs) was achieved employing spray pyrolysis (SP) and low-temperature sintering at 900 °C. In order to minimize polarization losses, the design, synthesis and processing of materials are required to achieve a competitive SOFC performance in the IT range (e.g. power density ~ 1 $W\cdot cm_{-2}$; electrode area specific resistance (ASR) $\leq 0.3\ \Omega\cdot cm_{2}$) [1]. The lowest ASR values are generally observed for nanosized materials with a large surface area, requiring optimization of synthesis and processing [2].

The ORR is highly dependent on the composition and microstructural characteristics of the cathode, including porosity, surface area and grain size [3]. SP-prepared materials offered improved microstructure with smaller particle size and higher porosity (extended triple phase boundary) in comparison to slurry-coated electrodes of analogous composition [4. Impedance spectroscopy of symmetrical NSC:CGO/CGO/NSC:CGO cells indicated a lower high-frequency response of the SP-prepared electrodes with lower overall polarization resistance (Rp), attributable to improved charge-transfer at the electrode-electrolyte interface. Further reduction in Rp was achieved on decoration of the composite NSC:CGO electrodes with Ag NPs; the decorated composites were characterized by high resolution transmission electron microscopy (HRTEM) and high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM). Ag K-edge X-ray Absorption Near Edge Structure (XANES) and Extended X-ray Absorption Fine Structure (EXAFS) of CGO:Ag spray-pyrolyzed composites indicated that the Ag nanoparticles exhibit a core-shell structure with a Ag2O outer layer calculated to be two unit cells in thickness. The outer particle shell is suggested to participate in enhanced oxygen diffusion and electrochemical response, producing a diminished low-frequency contribution to the impedance polarization response of symmetrical cells below 700 ºC [5]. Anode-supported single-cell fuel cells of configuration NiO-

CGO/YSZ/CGO/NSC:CGO:Ag with a thin YSZ-CGO electrolyte provided a maximum power density of 0.6 W·cm^{-2} at 700 ºC.

References

[1] Gao, Z., et al., *A perspective on low-temperature solid oxide fuel cells.* Energy & Environmental Science, 2016. **9**(5): p. 1602-1644.
[2] Tsipis, E.V. and V.V. Kharton, *Electrode materials and reaction mechanisms in solid oxide fuel cells: a brief review.* Journal of Solid State Electrochemistry, 2008. **12**(9): p. 1039-1060.
[3] Kan, W.H., A.J. Samson, and V. Thangadurai, *Trends in electrode development for next generation solid oxide fuel cells.* Journal of Materials Chemistry A, 2016. **4**(46): p. 17913-17932.
[4] Muñoz-Gil, D., et al., *The Effects of Sr Content on the Performance of Nd1–xSrxCoO3−δ Air-Electrode Materials for Intermediate Temperature Solid Oxide Fuel Cells under Operational Conditions.* Inorganic Chemistry, 2020. **59**(17): p. 12111-12121.
[5] Chen, J., et al., *One-pot synthesis of thermally stable gold@mesoporous silica core-shell nanospheres with catalytic activity.* Nano Research, 2013. **6**(12): p. 871-879.

W1-O10. Comments on the suitable hydrogen storage materials for vehicular applications

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Hydrogen storage in solid state metal hydride systems is the most efficient and safest way for storing hydrogen for vehicular applications [1]. A metal hydride filled on-board hydrogen fuel tank needs to be developed for H_2 vehicles, to (i) reversibly accommodate over 4 kg hydrogen on-board, preferably with respect to a total weight of 100 kg system (roughly 70 kg hydride + 30 kg system components) (ii) allow the refilling within 3-5 minutes, (iii) operate within 5-12 bar at a maximum temperature of 85 °C. Keeping these in view, several hydrogen storage materials were investigated but only three classes (i) intermetallic hydrides (e.g, $LaNi_5H_6$), (ii) complex hydrides (e.g $NaAlH_4$) and (iii) binary hydrides (e.g MgH_2) show the merit for experimental trials. Moreover, each material show some potential challenges, for instance (i) $LaNi_5H_6$ (intermetallic hydride) work better in lower temperature / pressure conditions, but they can accommodate a theoretical maximum of 0.97 kg hydrogen per 70 kg of storage material (experimentally, |~0.7 kg), (ii) $NaAlH_4$ (complex hydride), accommodates theoretically 3.85 kg (experimentally, ~0.28 kg) with the operational conditions of 200 °C/60 bars and (iii) MgH_2 (binary hydride) accommodates theoretically 5.32 kg hydrogen per 70 kg hydride (experimentally, ~4.2 kg), with the operational requirement of 320 °C/6 bar H_2. Presently the third option, i.e, MgH_2, seems to be the choice but considerable efforts are required for decreasing the dehydrogenation temperature and improving the kinetics of the system. Approaches like nano catalysis and nanoconfinement are being made by worldwide researchers and several encouraging developments have resulted across the world [2]. Based upon the experimental works carried out in our laboratory, in our opinion, magnesium hydride and the magnesium hydride - lithium borohydride reactive hydride composite are the most futuristic materials for vehicular applications.

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References

[1] Pukazhselvan, D., Kumar, V., & Singh, S. K. (2012). *Nano Energy*, *1*(4), 566-589.
[2] Yang, J., Sudik, A., Wolverton, C., & Siegel, D. J. (2010). *Chemical Society Reviews*, *39*(2), 656-675.

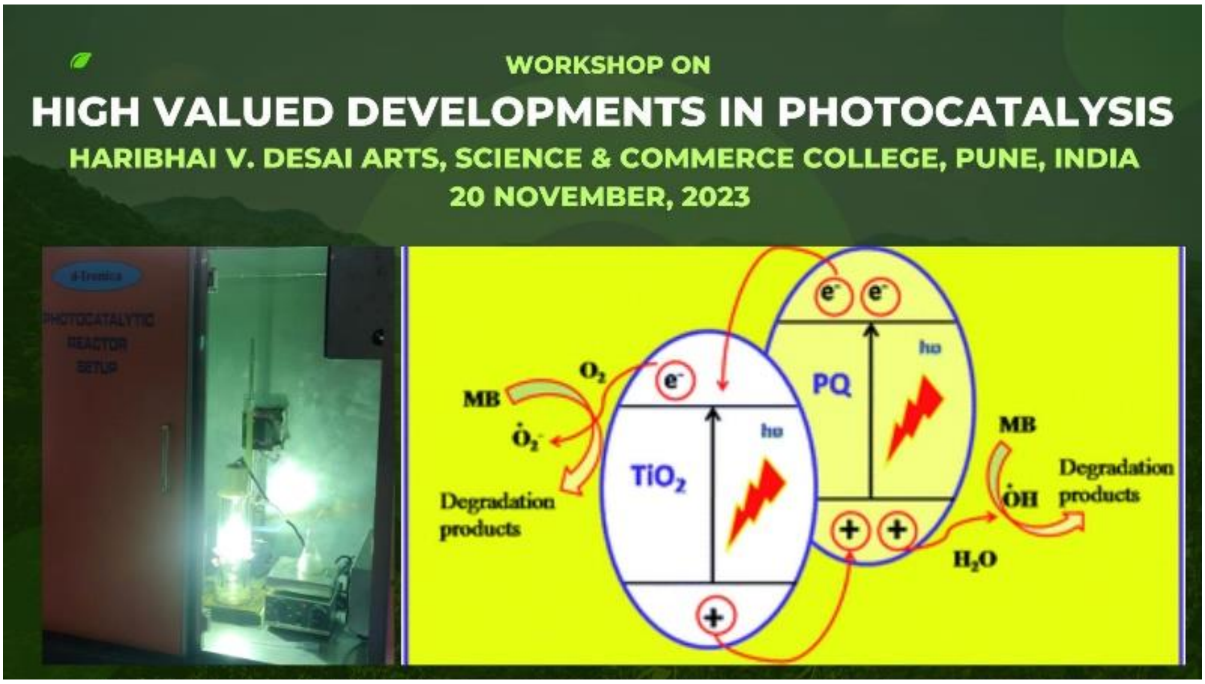
Workshop 2

WORKSHOP ON

HIGH VALUED DEVELOPMENTS IN PHOTOCATALYSIS

HARIBHAI V. DESAI ARTS, SCIENCE & COMMERCE COLLEGE, PUNE, INDIA

MONDAY, 20TH NOVEMBER, 2023



WORKSHOP ON

HIGH VALUED DEVELOPMENTS IN PHOTOCATALYSIS

HARIBHAI V. DESAI ARTS, SCIENCE & COMMERCE COLLEGE, PUNE, INDIA

20 NOVEMBER, 2023

WHVDP-2023 focuses on Great achievements in Photocatalysis field in order 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

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Workshop Website: https://icntri2023.nmsme.org/icntri2023/workshop-2/

Workshop on High Valued Developments in Photocatalysis
Haribhai V. Desai Arts, Science & Commerce College, Pune, India,20 November, 2023
Auditorium 3

9:40 - 10:00	**WELCOME ADDRESS** **Dr. Vikram U. Pandit,** **Dr. Rajendra G. Gurao**
10:00 - 10:30	**W2-IT1** **Prof. Ganesh Jadhav** *Haribhai V. Desai College, Pune, India* **Water Purification using Ex-situ Catalyst system**
10:30 - 11:00	**W2-IT2** **Prof. Vivekanand Jawale** *RKM College, Akurdi, Pune, Maharashtra 411035, India* **Dye Degradation using Organic Inorganic Catalyst.**
11:00 - 11:30	***W2-IT3*** **Dr. Sachin Wadhai** ***Savitribai Phule Pune University, Pune, India*** **Water Splitting**
11:30 - 12:00	**W2-QIT4** **Prof. Omkar Malusare** *H. V. Desai College, Pune India* **Water Purification using In-situ Catalyst system.**
12:00 - 12:40	**PP1: Bhagwan Daphal** **Synthesis, Characterization of Polyaniline and Polyaniline - V2O5 Nanocomposite for Photocatalytic Application** **PP2: Jatin Mithari** **Synthesis of Bismuth Oxyhalide (BiOX, X = I) Photocatalyst for waste water remediation** **PP3: Ganesh Dawange** **Photocatalytic applications of Copper Oxide, PQ and their composite in the degradation of organic dyes** **PP4: Purnima Patil** **An Efficient Visible Light Driven Bismuth Ferrite Incorporated 6,13-Pentacenequinone (BFO/PQ) Composite Photocatalytic Material for Degradation of Pollutants**

Workshop on High Valued Developments in Photocatalysis
Haribhai V. Desai Arts, Science & Commerce College, Pune, India,
20 November, 2023

PP1. Synthesis, Characterization of Polyaniline and Polyaniline - V_2O_5 Nanocomposite for Photocatalytic Application

Bhagwan Daphal, Vikram Pandit*

Department of Chemistry, Haribhai V. Desai College of Commerce, Arts and Science, Pune-411002, India

(Email: *vikramupandit@gmail.com*)

Polyaniline, a conducting polymer known for its electrical and optical properties, was synthesized through simple and cost-effective chemical oxidative polymerization method. The polyaniline was characterized using various techniques like Fourier-transform infrared spectroscopy (FTIR), UV-Visible spectroscopy and X-ray diffraction (XRD) to elucidate its structural and optical properties. Subsequently, polyaniline – V_2O_5 nanocomposite was prepared by the incorporation of V_2O_5 nanoparticles into the polyaniline matrix. The nanocomposite was characterized using similar techniques to evaluate its structural, morphological and optical properties. The synergistic effects between polyaniline and V_2O_5 in the nanocomposite were investigated to understand the potential enhancement of photocatalytic activity. The photocatalytic performance of both polyaniline and the nanocomposite was evaluated by studying the degradation of Rhodamine 6G under visible light irradiation. The results demonstrated that the polyaniline-V_2O_5 nanocomposite exhibited superior photocatalytic activity compared to polyaniline, suggesting the beneficial role of V_2O_5 nanoparticles in enhancing the photocatalytic efficiency.

PP2. Synthesis of Bismuth Oxyhalide (BiOX, X = I) Photocatalyst for waste water remediation

Jatin A. Mithari[1,2], Vikram U. Pandit[1*], Sucheta A. Gaikwad[2]

[1] Department of chemistry, Hari Bhai. V. Desai College, Pune, India

[2] Department of Chemistry, S. P. College, Pune, India

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In this study, highly photoactive BiOI nanoparticles (NPs) under sunlight irradiation were synthesized by a facile precipitation method using polyvinylpyrrolidone (PVP) at room temperature. Further as prepared catalysts were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM-EDX). Fourier transform infrared spectroscopy (FTIR). The results of XRD showed that PVP did not have any significant effect on crystalline structure of BiOI. Also, using different amounts of PVP in the synthesis led to different morphologies and sizes of BiOI particles. In addition, the photocatalytic activity of prepared photocatalyst was evaluated in the photodegradation of methylene blue dye under sunlight irradiation. The SEM (EDX) showed the crystalline morphology of BiOI which led to better surface area of the nanoparticle. The obtained results of dye degradation impart the role of particle size & surface area of prepared nanoparticles. SEM -EDX of the prepared BiOI indicates the presence of Bi, O, & I in various percentage. The photocatalyst of 6,13 pentacenequinone/BiOI with different weight ratios were prepared. The PQ/BiOI nanocomposite was prepared by using simple wet impregnation method. The prepared catalyst was characterized with various spectroscopic methods. The photocatalytic activity of coupled PQ/BiOI catalyst was studied by observing the degradation of methylene blue dye under visible light irradiation. As compared to the individual component, the coupled catalyst showed higher photocatalytic activity towards MB degradation.

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20 November, 2023

PP3. Photocatalytic applications of Copper Oxide, PQ and their composite in the degradation of organic dyes

Ganesh Dawange, [1,2] Mohan Sangale,[1] Vikram Pandit[3]

[1] *S.S.G.M. College,Kopargaon, India*

[2] *Sanjivani College of Engineering Kopargaon, India*

[3] *Haribhai V. Desai College, Pune, INDIA*

Photocatalysis is one of the efficient method and applied for the treatment of waste water. The PQ/CuO nanoparticles photocatalyst were prepared by wet impregnation method and its efficiency was assessed in the photocatalytic applications. The prepared PQ, CuO nanomaterials were characterized using XRD, FTIR, SEM and particle size analyzer. The degradation of Methylene blue (MB) and organic matters done by using different concentration amounts of CuO (0.5 – 4 % wt% of PQ). Effect of different parameters such as the concentration of CuO, amounts of the nanocomposite, pH, and concentrations of the (5, 10 ,20 ,50 ppm) MB solution and influence of sunlight radiation were examined. The results showed that 1% CuO/ PQ nanocomposite had the highest degradation efficiency of MB (81%) at 75 min, 1g/l of the nanocomposite is the best at pH 9, time 60 min, 5 mg.L^{-1} concentration of MB solution were suitable for removal of MB in both UV and sunlight radiation. It was found that the degradation efficiency increased as irradiation time increased. The degradation efficiency of CuO/ PQ nanocomposite against TOC, COD, and BOD was 100% for both surface and groundwater samples after 60 min. under UV and sunlight conditions.

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PP4. An Efficient Visible Light Driven Bismuth Ferrite Incorporated 6,13-Pentacenequinone (BFO/PQ) Composite Photocatalytic Material for Degradation of Pollutants

Purnima Patil [a], Vikram Pandit *

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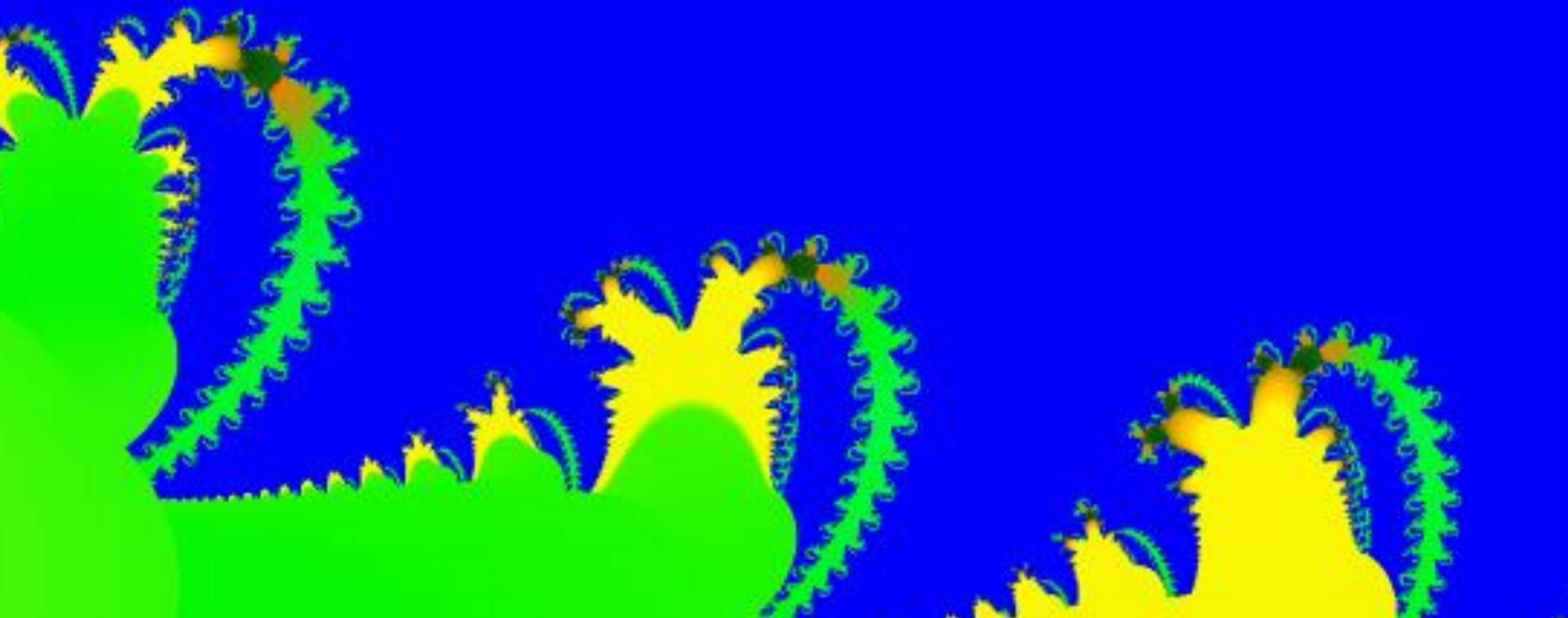
In recent times, the ever-increasing demands of fresh water have been stressing the need of developing and employing novel, efficient methods for water treatment. One of such methods that has been widely studied and applied for effective water and wastewater treatment is photocatalysis. Bismuth ferrite as a photocatalyst is known to demonstrate excellent magnetic properties, which can be effectively used for its easy separation from aqueous solution after wastewater treatment. An efficient (bismuth ferrite-pentacenequinone) BFO/PQ composite photocatalytic material was synthesized using simple wet impregnation process and its photocatalytic performances were evaluated by the photocatalytic degradation of Rhodamine B (RhB) in visible-light irradiation. The fabricated photocatalyst was analysed for in-depth understanding of its structural, light absorption and morphological features. The photodegradation efficiency results demonstrated that the BFO/PQ composite with 3% by weight loading displayed higher photocatalytic activity than various other PQ loadings, pristine BFO and PQ. The experiments of the photocatalytic degradation of RhB were conducted under natural sunlight, considering the band gap of the photocatalyst in the visible light.

Workshop 3

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

University of Aveiro,
Portugal,
20 November, 2023




Workshop New
Challenges of
Bionanomaterials:
Science, Technology,
Application

University of Aveiro,
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20 November, 2023

Modern state of Earth civilization show tendency with increase role of quality of people life. This is including, on the first-place, level of medicine, so, biology. In present days development of biomaterials, nano science and information technology give optimistic perspectives on this ~~way~~ direction and this allows more and more new horizons in Life sciences, Ecology, Green technologies, Education, Social organization society, etc. Thus, great opportunities open for young researchers in the realization they noble desires in understanding very difficult and very interesting fundamental laws of nature and to make practically a harmonious human future. Focusing, understanding and international exchange of knowledge are the basis for solving new questions in these areas. With this objective, we organize Workshop on Modern Problems of Bionanomaterials: Science, Technology, Application (WNCBM2023) with presentations and discussions specialists in Biomaterials, Nano science and Nano technology.

Workshop New Challenges of Bionanomaterials: Science, Technology, Application, University of Aveiro, Portugal, 20 November, 2023

Topics:

Bio-nanofabrication
Nanostructured Materials
Nanoassemblies / Surfaces
Modelling of Bionanomaterials
Bio-Inspired nanomaterials
Bio-nano measurement and microscopy
Nanobioanalysis in vitro
Nanotoxicology
Nanotechnology safety
Nanomaterials for Medicine and Medical Diagnostics
Body Implants and Prosthesis
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Nanosurfaces and Interactions
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November 20, 2022 (Monday)

12:15 – 14:00	Lunch break
	Workshop on New Challenges of Bionanomaterials: Science, Technology, Application University of Aveiro, Portugal, 20 November, 2023
14.00 - 14:20	**WELCOME ADDRESS** Dr. Igor Bdikin, Dr. Alejandro Heredia Barbero, …
14:20 - 14:50	CHAIRS: Gil Alberto Batista Gonçalves ***Invited talk (W3-I1)*** **Levodopa-Functionalized Gold Nanourchins as Highly Efficient Nanosensors for Detecting Contaminants** Prof. Dr. Ricardo João Borges Pinto *Department of Chemistry, University of Aveiro, Portugal*
14:50 - 15:10	***W3-O1*** **Gold nanoparticles (Eco)toxicity** Valérie Carvalho *Department of Biology, University of Aveiro, Portugal*
15:10 - 15:30	***W3-O2*** **Comparative assessment of the cytotoxicity of fuel- and bio-based micro(nano)plastics: amphibian cells as biological models** Carolina Frazão *Department of Biology, University of Aveiro. Portugal*
15:30 – 15:40	**Coffee break / Open discussions**
15:40 - 16:00	***W3-O3*** **Bovine Serum Albumin Nanoparticles as Drug Delivery Systems for Prostate Cancer Treatment** Dr. Beatriz Teixeira *Department of Biology, University of Aveiro, Portugal*
16:00 - 16:50	***W3-O4*** **Atomic force microscopy of organic microstructures** Dr. Igor Bdikin *Department of Mechanical Engineering, University of Aveiro, Portugal*
16:50 - 17:00	**Final discussion and comments**

Workshop on New Challenges of Bionanomaterials: Science, Technology, Application
University of Aveiro, Portugal, 20 November, 2023

W3-I1. Levodopa-Functionalized Gold Nanourchins as Highly Efficient Nanosensors for Detecting Contaminants

Marina Justi[1], Sara Fateixa[1], Violeta A. Girão[1], Mónica Almeida[2], Miguel Oliveira[2], João A. P. Coutinho[1], Ana M. Ferreira[1], **Ricardo J.B. Pinto[1,*]**

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In recent years, innovative materials have advanced food safety with faster detection of additives and contaminants. Gold nanoparticles (AuNPs) are key in this field, notably for their use as nanosensors, e.g., utilizing surface-enhanced Raman spectroscopy (SERS). Anisotropic morphologies, like nanourchins (AuNUs), outperform isotropic nanoparticles due to their branched structure and "hot points" with strong electromagnetic fields. However, it is crucial to develop eco-friendly methods for precise control over size and morphology in obtaining these Au anisotropic nanostructures while demonstrating that they are safe and effective in detecting various contaminants. In this study, we synthesized for the first time Au nanostructures, viz. nanourchins, using *Mucuna pruriens* levodopa extract and assessed their capability for detecting food contaminants. We investigated the effect of several reaction parameters, namely the use of polyethylene glycol (PEG), gold seeds, gold salt, and levodopa extract concentration, to control AuNPs' morphology and size. We found that a low seed volume and high levodopa concentration resulted in larger AuNUs, while a high seed volume and low levodopa concentration resulted in spherical shapes. Balanced seed and levodopa conditions produced smaller AuNUs without protrusions. Afterwards, the three AuNUs samples were evaluated for their effectiveness in detecting methylene blue, a toxic food additive, and rhodamine B, a common toxic dye. All gold nanostructures successfully detected both compounds, with the small AuNUs exhibiting the strongest SERS signal. These findings highlight the potential of these biobased gold nanostructures for creating efficient nanosensors to detect specific food additives and contaminants.

Acknowledgments

This work was partly developed within the scope of the project CICECO-Aveiro Institute of Materials, UIDB/50011/2020, UIDP/50011/2020 & LA/P/0006/2020, financed by national funds through the FCT/MCTES (PIDDAC). AMF acknowledges FCT for the CEECIND/00361/2022 contract under the Scientific Stimulus – Individual Call. The research contract of R.J.B. Pinto was funded by national funds (OE), through FCT in the scope of the framework contract foreseen in the numbers 4, 5, and 6 of the article 23, of the Decree-Law 57/2016, of August 29, changed by Law 57/2017, of July 19.

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University of Aveiro, Portugal, 20 November, 2023

W3-O1. Gold nanoparticles (Eco)toxicity

Valérie Carvalho[1,*], Miguel Oliveira[2], Mónica Almeida[2]

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Gold nanoparticles have been widely used in several areas of human activities, including biomedical field, due to their small size and unique properties [1]. However, with the increased use of these particles its entrance into the environment may be expected. There is thus the need to understand how the nanoparticles used in biomedical applications will affect environmental health, and ultimately human health. One of the prerequisites for using gold nanoparticles is their non-toxic and biocompatible nature to both *in vivo* and *in vitro* systems [2]. However, some concerns on their possible impact in the environment have been risen with few studies addressing the effects of the particles in marine organisms [3]. This work will present data on the biochemical effects of gold nanoparticles in marine organisms (bivalves and fish), alone and combined with other environmental contaminants. Overall, data show that the particle stability in high ionic strength media and the observed effects are highly dependent on the surface coating. Nonetheless, nanoparticles proved able to induce peroxidative damage both in bivalves and fish and promote alterations in neurotransmission. Although the benefits of these nanomaterials are widely proven, their unintentional release or disposal deserve more care and precaution.

References

[1] Dykman LA, Khlebtsov NG. Gold nanoparticles in biology and medicine: recent advances and prospects. Acta Naturae. 2011 Apr;3(2):34-55. PMID: 22649683; PMCID: PMC3347577
[2] Sani A, Cao C, Cui D. Toxicity of gold nanoparticles (AuNPs): A review. Biochem Biophys Rep. 2021 Apr 10;26:100991. doi: 10.1016/j.bbrep.2021.100991. PMID: 33912692; PMCID: PMC8063742.
[3] Teles A, Reyes-López FE, Balasch JC, Tvarijonaviciute A, Guimarães L, Oliveira M, Tort L. Toxicogenomics of Gold Nanoparticles in a Marine Fish: Linkage to Classical Biomarkers. Front. Mar. Sci. 6:147. doi: 10.3389/fmars.2019.00147

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W3-O2. Comparative assessment of the cytotoxicity of fuel- and bio-based micro(nano)plastics: amphibian cells as biological models

Carolina Frazão[1, *], Mónica Almeida[1], Miguel Tamayo-Belda[2], Ricardo J.B. Pinto[3], Isabel Lopes[1], Miguel Oliveira[1]

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The low cost, versatility, and durability of plastic materials led to its increased production [1], resulting in its environmental presence. Once in the environment, abiotic and biotic processes may lead to their degradation/fragmentation down to microplastics (MP < 5 mm) and nanoplastics (NP < 100 nm) [2]. A decrease in size often increases the bioavailability and reactivity of the particles. Ethical constraints limit the tests that can be employed to understand the hazards of MP and NP to vertebrates, including amphibians. Amphibians are under anthropogenic pressure worldwide, therefore *in vitro* cellular models based on established cell lines are of great significance for the risk assessment of MP and NP to vertebrates [3]. The increased concern over plastic pollution led to a shift in the plastic industry towards the development of bioplastics (e.g., polylactic acid). Whether bio-based plastics are more eco-friendly than conventional fuel-based is still to be proved. Despite their reported biodegradable nature, when disposed of in an uncontrolled fashion, bio-based plastics will accumulate in the environment and fragment into MP and NP [4]. There is a lack of information on the effects of different polymers, especially on freshwater organisms (e.g., amphibians). This study aimed to evaluate the cytotoxic effects of micro(nano)plastics in amphibian cell lines. In this study, two amphibian cell lines were selected, A6 (adult *Xenopus laevis* kidney epithelial cell line) and XTC-2 (tadpole *Xenopus laevis* carcass fibroblast cell line). Nanoparticles of polymethylmethacrylate (PMMA, fuel-based) with and without fluorescence (perylene) were synthesized by mini-emulsion polymerization of methyl methacrylate with sodium dodecyl sulfate (SDS) as a stabilizer [5]. Polystyrene (PS, fuel-based) and polylactic acid (PLA, bio-based) were obtained through fragmentation. The PMMA particles were characterized by dynamic light scattering (DLS). Viability assays showed no significant effects on A6 after exposure to PMMA with and without perylene, while when exposed to PLA a reduction in viability was observed at the tested highest concentration (200 mg/L).

XTC-2 had a reduction of viability at the highest concentration of PMMA (400 mg/L) with perylene and PLA (200 mg/L) and no effects to PS.

Acknowledgments

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References

[1] Q. Zhang, EG. Xu, J. Li, Q. Chen, L. Ma, EY. Zeng, et al., *Environ Sci Technol,* 54, 3740-51 (2020).
[2] M. Oliveira, M. Almeida, *TrAC - Trends Anal Chem*, 114, 196-201 (2019).
[3] Q. Shi, J. Tang, R. Liu, L. Wang, *Crit Rev Environ Sci Technol*, 1-33 (2021).
[4] VC. Shruti, G. Kutralam-Muniasamy, *Sci Total Environ*, 697, 134139 (2019).
[5] P. Manuel, M. Almeida, M. Martins, M. Oliveira, *Environ Res,* 213 (2022).

W3-O3. Bovine Serum Albumin Nanoparticles as Drug Delivery Systems for Prostate Cancer Treatment

Beatriz Teixeira[1,*], Sónia A.O. Santos[2], Mónica Almeida[3], Miguel Oliveira[3], Ricardo J.B. Pinto[2]

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Cancer is a major health challenge worldwide, placing a burden on healthcare systems and leading to high mortality rates. Prostate cancer, the second most common cancer in males, has a high incidence and mortality rate. Current treatments, including surgery, radiation, hormone therapy, and chemotherapy, are often associated with side effects and limitations such as lack of specificity and chemotherapy resistance.[1] To overcome these limitations, scientists are exploring alternative, more precise therapies. One promising avenue is the use of polymeric nanoparticles (NPs) for drug delivery.[2] In particular, protein-based NPs offer advantages such as environmentally friendly production, stability, and biocompatibility.[2,3] However, challenges still exist, such as improving NP uniformity, avoiding toxic substances such as glutaraldehyde, improving drug loading, and evaluating clinical viability.

In this study, we prepared bovine serum albumin (BSA) nanoparticles (NPs) using genipin crosslinking for drug encapsulation. We investigated the effects of temperature, stirring method, and BSA/genipin concentrations on NP size, stability, and yield. The ideal size of BSA NP for cell-based *in vitro* assays (≈300 nm) was achieved at the same BSA and genipin concentrations (20 mg/mL) (Figure 5). Higher reaction temperatures increased yield but affected size and aggregation. We successfully encapsulated clinical drugs (sertraline and 5-fluorouracil), with BSA NPs showing high sertraline loading (82% via HPLC-MS). *In vitro* tests on normal and prostatic carcinoma cell lines confirmed BSA NPs as promising nanocarriers for the treatment of prostate cancer.

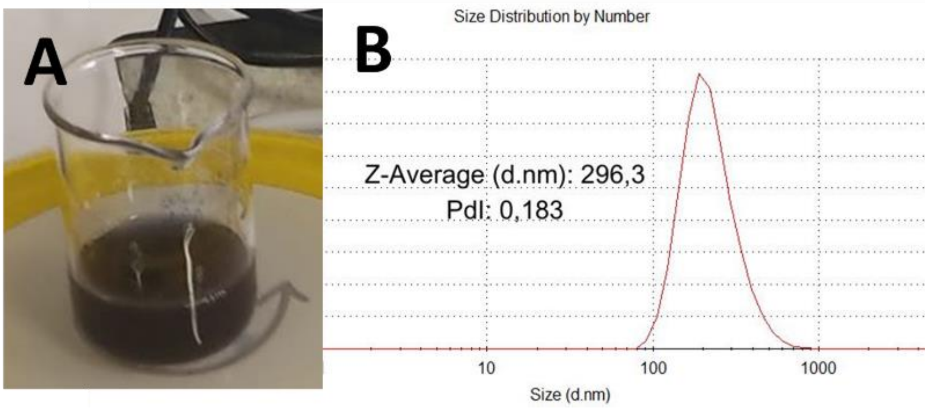

Figure 5: A) Aqueous suspension of BSA NPs and B) respective hydrodynamic diameter.

Acknowledgements: This work was partly developed within the scope of the project CICECO-Aveiro Institute of Materials, UIDB/50011/2020, UIDP/50011/2020 & LA/P/0006/2020, financed by national funds through the FCT/MCTES (PIDDAC). The research contract of R.J.B. Pinto was funded by national funds (OE), through FCT in the scope of the framework contract foreseen in the numbers 4, 5, and 6 of the article 23, of the Decree-Law 57/2016, of August 29, changed by Law 57/2017, of July 19. Thanks are due to FCT/MCTES for the financial support to the project NanoPlanet (2022.02340.PTDC), the research contract under Scientific Employment Stimulus to S.A.O. Santos (2021.03348.CEECIND), and CESAM (UIDP/50017/2020+UIDB/50017/2020+LA/P/0094/2020) through national funds.

References

[1] M. Sekhoacha, K. Riet, P. Motloung, L. Gumenku, A. Adegoke and S. Mashele, Molecules, 2022, 27, 5730.
[2] Y. Miao, T. Yang, S. Yang, M. Yang and C. Mao, Nano Converg, 2022, 9, 2.
[3] M. J. Mitchell, M. M. Billingsley, R. M. Haley, M. E. Wechsler, N. A. Peppas and R. Langer, Engineering precision nanoparticles for drug delivery, Nat Rev Drug Discov, 2020, 20, 101.

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W3-O4. Atomic force microscopy of organic microstructures

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

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

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

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

Workshop 4

Colloquium on

Advances in materials for sustainability (online)

20 November 2023

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Probing techniques in nanostructures
Catalysis and environmental aspects
Electrical measurements, instrumentation, and characterization methods

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Colloquium on Advances in materials for sustainability
University of Aveiro, Portugal, 20 November, 2023

9.20 - 9:30	**WELCOME ADDRESS** Dr. Eskilla Venkata Ramana and Dr. Indrani Coondoo
09:30 – 10:30	**Dr Jiri Rathorsky (Invited)** **Photocatalytic degradation of aqueous pollutants** **J. Heyrovský institute of physical chemistry of the CAS, Prague, Czech Republic**
10:30 – 11:15	**Dr Xiao Long (Invited)** **Non-volatile optically controlled BTO ferroelectric tunnel junctions and CMOS compatible volatile HZO ferroelectric tunnel junctions** **Institute of Microelectronics, Chinese Academy of Sciences, Beijing, China**
11:15 – 12:00	**Dr V Raghavendra Reddy (Invited)** **UGC-DAE, Indore, India** **Magnetism in ferroelectric four-layered Aurivillius $Bi_5FeTi_3O_{15}$ compound**
12:00 – 12:20	**Daniela Santos (Oral)** **Universidade do Minho, Braga, Portugal.** **Functionalized Nanofibers with Cyclodipeptides for Thermal Sensing and Energy Harvesting**
12:20 – 12:40	**Bruna M. Silva (Oral), Universidade do Minho, Braga, Portugal.** **Strain dependent magnetic and dielectric properties of Ca3Mn2O7 thin films prepared by pulsed laser deposition**
12:40 – 13:00	**Vishakha Sharma (Oral)** **DTU, India** **Metalens Magic-Shaping the Future of nanostructure probing**
13:00 - 14:30	Lunch break
14:30 – 15:15	**Dr Buchi Suresh (Invited)** **International advanced research centre for powder metallurgy (ARCI), Hyderabad, India.** **Solid Oxide Cells (SOFC/SOEC): An energy efficient clean and green technology for the production of energy and hydrogen**
15:15 – 15:35	**Dr. V.C. Bharath Sabarish (oral)** **K. Ramakrishnan College of Technology, Trichy, India** **Effect of particles/ions irradiation on Triglycine sulphate single crystal on its ferroelectric and piezoelectric properties**

W4-O1. Nanofibers Functionalized with Cyclodipeptides for Thermal Sensing and Energy Harvesting

Daniela Santos *, Rosa Baptista, Etelvina de Matos Gomes, Bernardo Almeida

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Biological building blocks, particularly dipeptides, have the ability to self-assemble into well-organized structures with functional properties, making them valuable in both biology and nanotechnology. Designed dipeptide building blocks self-assemble into diverse nanostructures like nanotubes, vesicles, fibrils, and wires, enhancing their properties and versatility. These nanostructured dipeptide assemblies, with quantum confinement, hold promise in materials science as eco-friendly optoelectronic materials for energy harvesting, thanks to their biocompatibility, ease of fabrication, and functionalization.

Cyclic dipeptides, specifically aromatic cyclo-dipeptides with tryptophan, are versatile nanomaterials with remarkable properties. They self-assemble into various supramolecular structures like nanospheres, nanotubes, and nanowires, exhibiting quantum confinement and photoluminescence. Chiral cyclic dipeptides can even demonstrate piezoelectric and pyroelectric properties, offering potential applications in nano energy sources. These dipeptides, known for their high thermal stability and mechanical strength, are incorporated into biopolymer matrices through electrospinning to create nanofiber systems.

As such, here we report the fabrication of hybrid systems based on chiral cyclo-dipeptide L-Tryptophan-L-Tryptophan and cyclo-L-Tryptophan-L-Tyrosine incorporated into biopolymer electrospun fibers [1,2]. The micro/nanofibers contain self-assembled nanostructures embedded into the polymer matrix, are wide-band gap semiconductors with 4.0 eV bandgap energy, and display blue photoluminescence as well as relevant piezoelectric and pyroelectric properties. A piezoelectric nanogenerator was proposed, tested and shown to be capable of producing 0.18 μWcm^{-2} of power density and have a piezoelectric coefficient of 57 pCN^{-1} for Cyclo (L-Trp-L-Trp)@PLLA. Therefore, the fabricated hybrid mats are promising systems for future thermal sensing and energy harvesting applications [1].

References

[1] D. Santos, R. Baptista, A. Handa, B. Almeida, P. Rodrigues, A. Torres, A. Machado, M. Belsley and E. de Matos Gomes, *Materials*, **16(6)**, 2477 (2023).

[2] D. Santos, R. Baptista, A. Handa, B. Almeida, P. Rodrigues, C. Castro, A. Machado, M. Rodrigues, M. Belsley and E. de Matos Gomes, *Materials*, **16(14)**, 4993 (2023).

Colloquium on Advances in materials for sustainability
University of Aveiro, Portugal, 20 November, 2023

W4-O2. Strain dependent magnetic and dielectric properties of $Ca_3Mn_2O_7$ thin films prepared by pulsed laser deposition

B. M. Silva[1, *], J. Oliveira[1], V. Lenzi[1], P. Rocha-Rodrigues[2], P. Neenu Lekshmi[2], L. S. Marques[1], A. M. L. Lopes[2], J. P. Araújo[2], B. G. Almeida[1]

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Naturally Layered Perovskite structures with improper ferroelectricity, such as the Ruddlesden-Popper calcium manganite compound $Ca_3Mn_2O_7$, offer an alternative route to achieve non-expensive and high-performance room-temperature multiferroic magnetoelectricity. They allow exploring oxygen octahedra nonpolar rotations and cation site displacement to attain non-centrosymmetry. Additionally, their high sensitivity to lattice distortions allows for the manipulation of acentricity through preparation as thin films over crystalline substrates, which enables tuning of lattice, electric, and magnetic interactions [1]. As such, thin films of $Ca_3Mn_2O_7$ with variable thicknesses were prepared by pulsed laser deposition over (100) $SrTiO_3$ substrates and their structural, dielectric and magnetic properties were characterized [2].

The $A2_1am$ ferroelectric phase was observed in the films, along with the orthorhombic Acaa phase. The X-ray diffraction results show stronger strain in the thinner films that progressively relaxed with increasing sample thickness. The magnetic properties show the presence of an antiferromagnetic (AFM) transition between 90 and 110 K.

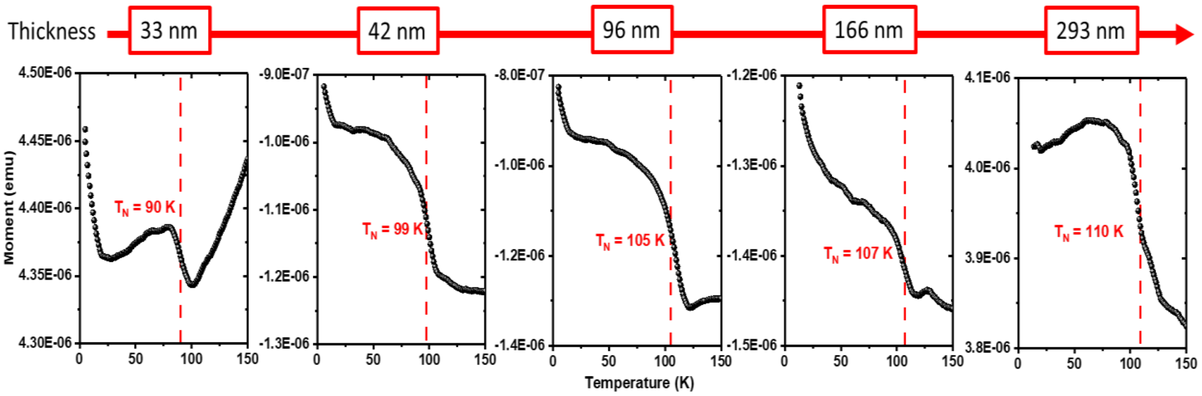

Figure 1: Temperature dependence of the magnetization measured in $Ca_3Mn_2O_7$ thin films with increasing thickness over $SrTiO_3$ substrates and their corresponding AFM transition temperatures.

The dielectric permittivity of the films shows the presence of dispersion described by the Havriliak-Negami model function with two relaxations. From temperature-dependent fits to the permittivity curves, different behavior of the parameters was observed above and below the antiferromagnetic phase transition. The dielectric properties show the presence of an AFM transition between 85 and 112 K.

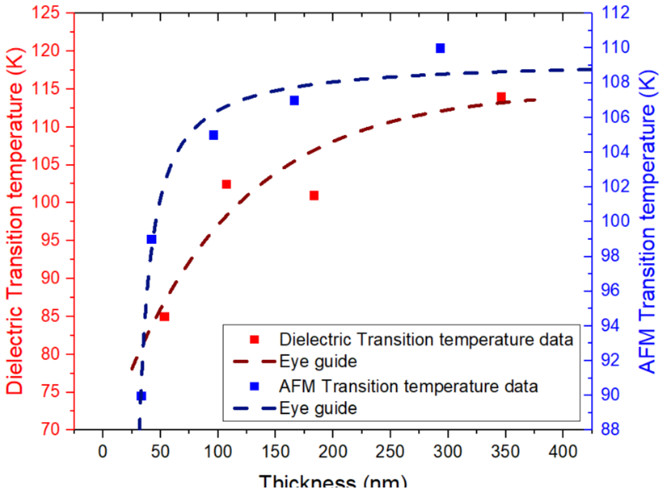

Figure 2: Comparison of AFM transition temperatures obtained through magnetic measurements (blue) with dielectric measurements (red).

Considering the results of magnetic and dielectric measurements, the AFM transition temperature was lower for more strained films and increases as the strain of the films decreases. For the thicker, less strained, film, with around 350 nm, an AFM transition at 110-112 K was found which is bulk $Ca_3Mn_2O_7$ Ruddlesden-Popper phase characteristic temperature. The magnetic/dielectric correlation results indicate the presence of magnetoelectric interactions and magnetically induced enhancement of dipolar-correlations in the AFM phase. In this work, a study of the strain-dependent magnetic and dielectric properties of the films produced will be discussed and presented.

References

[1] P. Ghosez and J. M. Triscone, Nat. Mater. **10**, 269 (2011).

[2] B. M. Silva, J. Oliveira, T. Rebelo, V. B. Isfahani, P. Rocha-Rodrigues, N. Lekshmi, J. H. Belo, F. L. Deepak, A. M. L. Lopes, J. P. Araújo, and B. G. Almeida, Mater. Res. Bull. **158**, (2023).

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The Centre for Mechanical Technology and Automation (TEMA) has been pursuing excellence, cutting-edge research and innovation since 1996. It is the main research interface of the Department of Mechanical Engineering, aligned to University of Aveiro commitment for innovation, quality, and international recognition in the areas of Engineering Education, Research and Cooperation with Society.

TEMA is focused on current societal challenges and upcoming global requirements, translated into three main mobilizing projects (MP): Mobilizing Project 1 – Sustainable Manufacturing Solutions; Mobilizing Project 2 - Technologies for the Wellbeing; and Mobilizing Project 3 - Research Infrastructure, involving TEMA's members as one coherent group. MP1 is focused on the development and innovation on manufacturing engineering and technologies, with subsequent industrial applications. It is intended to increase productivity, improve products'quality and reduce waste in production processes. The strategy of the MP2 aims to increase the quality of life of society by means of engineering systems, focusing on people and their needs. MP3 aims at a rational and efficient management of TEMA's material and human resources (including its 14 laboratories), its vast array of scientific equipment in a large diversity of areas available to society, making the research infrastructure an "open facility" for several (academic, research and industry) end-users.

TEMA is also actively working on the new Intelligent Systems Associate Laboratory (LASI). TEMA was part of the creation of LASI, which consists of 13 Research Units.

LASI establishes five inter-disciplinary research thematic lines to give response to social, scientific, health, sanitary, social, economic, and environmental challenges. The goal is to pave the next generation of knowledge and technologies for the development and transformation of the industry and society. In fact, each thematic line aims to tackle specific societal challenges. Innovative and Sustainable Industries is a thematic line that focuses on advanced manufacturing, decarbonization, factories of future, green AI, Industry 5.0, intelligent materials and products, and collaborative robotics. On the other hand, Smart Cities, Mobility and Energy aims to promote sustainable and green cities, focusing on urban computing, intelligent transportation systems, e-Citizenship as well as intelligent environments. The Health and Well-being thematic line focuses on active ageing, ambient assisted living, and smart intervention with personalized health, biomedical informatics, and medical robotics. Infrastructures and Highly Connected Society aims to tackle all society specific challenges based on methods and techniques that include cyber security, quantum computing, computational support, internet of things, and virtualization. Finally, the Public Administration and Governance research line focuses on E-governance, digital transformation, ethics, data protection and privacy, e-Services, and fair and effective governance.

Prof. Dr. António Manuel de Bastos Pereira
Director of TEMA - Centre for Mechanical Technology and Automation

Notes

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