# 5th International Conference on Nanomaterials Science and Mechanical Engineering

## University of Aveiro, Portugal

## July 5-8, 2022

# Book of Abstracts

tema
university of aveiro
centre for mechanical technology and automation

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# (5th ICNMSME-2022)

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

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http://icnmsme2022.web.ua.pt/

# ICNMSME2022 program

## July 5, 2022 (Tuesday)

| Workshop on Thin Films: Growth, Characterization, Application<br>University of Aveiro, Portugal<br>July 5, 2022<br>Auditorium 1 | | | Workshop on Optical Materials and their applications<br>University of Aveiro, Portugal,<br>July 5, 2022<br>Auditorium 3 | |
|---|---|---|---|---|
| 9:00 - 9:15 | **WELCOME ADDRESS**<br>Prof. Dr. Duncan Paul Fagg, Dr. Igor Bdikin | | 9.00 - 9:15 | **WELCOME ADDRESS**<br>Dr. Suresh Kumar Jakka, Dr. Pavani Krishnapuram and Dr. Igor Bdikin |
| 9:15 - 10:15 | Chair: Prof. Dr. Duncan Paul Fagg<br>***Plenary Lecture***<br>**Deposition of complex oxide thin films by multitarget reactive sputtering**<br>Prof. Dr. Gunnar Suchaneck<br>*Solid State Electronics Laboratory, Dresden University of Technology, Germany* | | 9:15 - 10:15 | Chair: Dr. Suresh Kumar Jakka<br>***Plenary Lecture***<br>***W4-PL1***<br>**New advances in rare earth based pressure and temperature optical sensors**<br>Prof. Victor Lavin<br>*Laser and High Pressure Spectroscopy group, University of La Laguna, Tenerife, Spain* |
| 10:15 – 11:15 | ***Plenary Lecture***<br>**Deposition of diamond films by chemical vapor deposition**<br>Dr. Joana Catarina Mendes<br>*Instituto de Telecomunicações AVEIRO, PORTUGAL* | | 10:15 - 10:45 | ***Invited talk***<br>***W4-IT1***<br>**Development of new emitting optical fibers for mid-Infrared applications**<br>Dr. Arnaud Lemiere<br>*Photonic Glasses group, Tampere University, Finland* |
| | | | 10:45 - 11:15 | ***Invited talk***<br>***W4-IT2***<br>**Multifunctionality of Fluorescent 2D-BCNO Sheets**<br>Dr. Venkatramaiah<br>*SRM university, Chennai, India* |
| 11:15 – 11:30 | **Final discussions and comments / Coffee break** | | 11:15 – 11:30 | **Coffee break / Open discussions** |

| **Workshop on Modern Problems of Bionanomaterials: Science, Technology, Application University of Aveiro, Portugal July 5, 2022**<br><br>**Auditorium 1** | | **"SMARTELECTRODES" Workshop: Smart metallic and semiconductor materials: synthesis, characterization, applications and challenges University of Aveiro, Portugal, July 5, 2022**<br><br>**Auditorium 2** | | **Workshop on Optical Materials and their applications University of Aveiro, Portugal, July 5, 2022**<br><br>**Auditorium 3** | |
|---|---|---|---|---|---|
| | Chair: Dr. Gil Gonçalves | | Chairs: Prof. Henrikas Cesiulis, Dr. Natalia Tsyntsaru | | Chair: Dr. Suresh Kumar Jakka |
| **11:30 – 12:15** | W1-O1.<br>**Problems of atomic force microscopy of organic materials**<br>Dr. Igor Bdikin<br>*Department of Mechanical Engineering, University of Aveiro, Portugal* | **11:30 – 11:55** | ***Keynote presentation***<br>W3-O1.<br>**Development of technological electrodes/processes at EPT and TOPAZ companies within SMARTELECTRODES project**<br>Dr. Natalia Tsyntsaru,<br>*Vilnius University, Lithuania/ Institute of Applied Physics, Moldova* | **11:30 - 12:00** | ***Invited speaker***<br>***W4-IT3***<br>**How to modify luminescent properties of materials by changing its structure**<br>Dr. Bartosz Bondzior<br>*Photonic Glasses group Tampere University, Finland* |
| | | **11:55 – 12:20** | ***Keynote presentation***<br>W3-O2.<br>**Application of electrochemical impedance spectroscopy (EIS) for processes and systems characterization**<br>Prof. Dr. Henrikas Cesiulis<br>*Vilnius University / EPT , Lithuania* | **12:00 - 12:15** | Oral presentation<br>W4-OP1<br>**Photocatalytic degradation activity of SrTiO3 against Methylene Blue Dye**<br>Mr. D. PrakashBabu<br>*REVA university, India* |
| | | **12:20 – 12:45** | ***Keynote presentation***<br>W3-O5.<br>**$Mo_xS_y$-containing coatings for photo/electrochemical water splitting applications**<br>Dr. Ramunas Levinas<br>*Vilnius University, /FTMC , Vilnius, Lithuania* | **12:15 - 12:30** | Oral presentation<br>W4-OP2<br>**UV excited blue to green emitting Tb3+ activated sodium calcium metasilicate color tunable phosphor for luminescent devices**<br>Ms. Deepali<br>*Delhi Technological University, India* |
| | | | | **12:30 - 12:40** | Poster presentation<br>W4-PP1<br>**Magnetically retrievable photocatalysis for dye degradation**<br>Mr. Sachin Kulkarni<br>*REVA university, India* |

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| | | | | **12:40 - 12:50** | Poster presentation<br>W4-PP2<br>**Spectral investigation of thermally stable Eu3+ activated potassium tungstate tellurite glasses for epoxy-resin free visible red component of photonic device applications**<br><br>Mr. Vikas Sangwan<br>*Delhi Technological University, India* |
| | | | | **12:50 - 13:00** | Poster presentation<br>W4-PP3<br>**Study on Photocatalytic inactivation of bacteria and dye degradation by Ag/SiO2/ZnO based nanoparticles**<br><br>Ms. Jaya Choudhary<br>*REVA university, India* |
| **12:15 – 14:00** | Lunch break | **12:45 – 14:00** | Lunch break | **13:00 – 14:00** | Lunch break |
| **14:00 – 15:00** | Chair: Dr. Gil Gonçalves<br><br>***Plenary Lecture***<br><br>**Review on Modern Problems of Bionanomaterials: Science, Technology, Application**<br><br>Prof. Dr. José M.F. Ferreira<br>*Department of Materials and Ceramic Engineering (DEMaC), University of Aveiro, Portugal* | **14:00 – 14:25** | Chairs: Prof. Henrikas Cesiulis, Dr. Natalia Tsyntsaru<br>***Keynote presentation***<br><br>W3-O6.<br>**Nanomultilayer structures based on chalcogenide amorphous semiconductors: obtaining and applications**<br><br>Dr. Alexei Mesalchin<br>*Institute of Applied Physics, Chisinau, Moldova* | **14:00 - 15:00** | Chairs: Dr. Pavani Krishnapuram Prof. K. Upendra Kumar<br>***Plenary Lecture***<br>***W4-PL2***<br>**A Method of Designing Uniform Sized Phosphor Nanoparticles and Fabrication of an AC-Electroluminescent Device**<br><br>Prof. D. Haranath<br>*Luminescent Materials and Devices (LMD) group, Department of Physics, National Institute of Technology Warangal, INDIA* |
| | | **14:25 – 14:50** | ***Keynote presentation***<br><br>W3-O4.<br>**Functional properties of Fe-Ga alloys prepared by electrodeposition**<br><br>Dr. Aliona Nicolenco<br>*Marie Curie fellow, Universitat Autònoma de Barcelona, Spain/ Institute of Applied Physics, Moldova* | | |

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| **15:00 – 15:15** | **Final discussion and comments** | **14:50 – 15:15** | ***Keynote presentation***<br><br>W3-O7.<br>**Electrodeposited Co-Mo Composites with Titania for the Hydrogen Evolution Reaction**<br><br>Dr. Cheng Wang<br>*Microfabrica Inc, CA / Clarkson University, USA* | **15:00 - 15:30** | ***Invited speaker***<br>***W4-IT4***<br>**Ceramic Luminescents for solid-state lighting applications**<br><br>Dr. Bungala Jamalaiah<br>*RGUKT college of Engineering and Technology, Nandyal, India* |
| | | **15:15 – 15:40** | ***Keynote presentation***<br><br>W3-O3.<br>Electrodeposited Alloys for the Oxygen Evolution Reaction (OER)<br><br>Prof. Dr. Elizabeth Podlaha-Murphy<br>*Clarkson University, USA* | | |
| | | **15:40 – 15:50** | **Final discussions and comments** | **15:30 - 16:00** | ***Invited talk / thesis presentation***<br>***W4-IT5***<br>**Cholesteric Liquid Crystal Emulsions for the Application in Anticounterfeiting Technology**<br><br>Mr. Buchaiah Gollapelli<br>*Department of Physics, NIT Warangal, India* |
| | | | | **16:00 - 16:30** | ***Invited talk***<br>***W4-IT6***<br>**Engineering of Silver Nanoclusters in Photoluminescent glass**<br><br>Dr. Seshadri Meruva<br>*K.G Reddy college of Engineering and Technology, Hyderabad, INDIA* |
| | | | | **16:30 - 16:45** | Oral presentation<br>W4-OP3<br>**Excitation and concentration-dependent energy transfer analysis in Dy3+/Eu3+ co-doped potassium zinc borophosphate glasses for white light emission**<br><br>Dr. R. Ramaraghavulu<br>*Annamacharya Institute of Technology and Sciences, Rajampet, India* |

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| | | | | **16:45 - 17:00** | Oral presentation<br>W4-OP4<br>**Enhancement of Photoluminescence of CaSiO3:Eu3+ co-doped Dy3+ nanophosphor**<br><br>Prof. M. Madesh Kumar<br>*REVA University, India* |
| | | | | **17:00 - 17:15** | Oral presentation<br>W4-OP5<br>**Energy transfer and tunable emission from single phase triply doped Ca3Bi(PO4)3 phosphor for WLEDs**<br><br>Mr. Mukesh K. Sahu<br>*Delhi Technological University, India* |
| | | | | **17:15 - 17:30** | **Final discussion and comments** |

# July 6, 2022 (Wednesday)

| 5th International Conference on Nanomaterials Science and Mechanical Engineering (5th ICNMSME-2022) (*online*) | |
|---|---|
| 9:00-9:30 | **Auditorium 1**<br><br>**WELCOME ADDRESS**: Prof. Dr. Robertt Angelo Fontes Valente (UA, Portugal), Prof. Dr. Vítor António Ferreira da Costa (UA, Portugal), Prof. Dr. António Manuel de Bastos Pereira (UA, Portugal), Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques (UA, Portugal), Dr. Duncan Paul Fagg (UA, Portugal), Dr. Igor Bdikin (UA, Portugal), Dr. Gonzalo Guillermo Otero Irurueta (UA, Portugal), Dr. Gil Alberto Batista Gonçalves (UA, Portugal) |
| 9:30-10:30 | Session: **New Materials and Advanced Materials**<br>CHAIRS: Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques<br>Dr. Gil Gonçalves<br>***Plenary Lecture***<br><br>Prof. Dr. Senentxu Lanceros-Méndez<br>**Printable smart and multifunctional materials for a digital and sustainable transformation**<br>*BCMaterials, Basque Center for Materials, Applications and Nanostructures, UPV/EHU Science Park, 48940 Leioa, Spain*<br>*IKERBASQUE, Basque Foundation for Science, 48009 Bilbao, Spain* |
| 10:30-10:45 | Coffee break |
| 10:45-11:25 | **Auditorium 1**<br>Session: **Nanocomposite Materials**<br>CHAIRS: Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques<br>Dr. Gil Gonçalves<br>***Plenary Lecture***<br><br>Prof. Dr. José M.F. Ferreira<br>**Improvement of mechanical performance of nanocomposite materials through processing: the key role of uniform dispersion of reinforcing CNTs**<br>*Department of Materials and Ceramic Engineering (DEMaC), University of Aveiro, 3810-193, Aveiro, Portugal* |

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|---|---|---|
| 11:25-12:15 | Session: **Modeling of Nano-structures**<br>CHAIRS: Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques<br>Dr. Gil Gonçalves<br>***Plenary Lecture***<br>Prof. Dr. Manuel Melle-Franco<br>**The Computational Microscope: a Versatile Tool to Understand and Design Novel NanoMaterials**<br>*CICECO, Department of Chemistry, University of Aveiro, 3810-193,Aveiro, Portugal* | |
| 12:15-14:00 | Lunch | |
| 14:00-14:50 | **Auditorium 1**<br>Session: **Micro / Nano Materials**<br>CHAIRS: Dr. Duncan Paul Fagg,<br>Dr. Aliaksandr Shaula,<br>Dr. Igor Bdikin<br>***Plenary Lecture***<br>Prof. Dr. Gunnar Suchaneck<br>**Tunnel magnetoresistance in granular ferro(ferri)magnetic systems**<br>*Institute of Solid-State Electronics, TU Dresden, 01062 Dresden, Germany* | |
| 14:50-15:40 | Session: **Biomaterials**<br>CHAIRS: Dr. Duncan Paul Fagg,<br>Dr. Aliaksandr Shaula,<br>Dr. Igor Bdikin<br>***Plenary Lecture***<br>Prof. Dr. Vincent Ball<br>**Catechol and its analogues in hydrogels and in electrodeposited films**<br>*Université de Strasbourg, Faculté de Chirurgie Dentaire, 8 rue Sainte Elisabeth, 67000 Strasbourg, France*<br>*Institut National de la Santé et de la Recherche Médicale, Unité Mixte de Recherche 1121, 4 rue Eugène Boeckel, 67084 Strasbourg Cedex, France* | |
| 15:40-16:00 | Coffee break | |
| 16:00-16:40 | **Auditorium 1**<br>Session: **Micro / Nano Materials**<br>CHAIR: Dr. Aliaksandr Shaula<br>***Keynote talk***<br>Dr. Pankaj Bharmoria **(I3)**<br>**Photonics Bioplastic Films for Triplet Sensitized Wideband Photon Harvesting**<br>*Department of Chemistry and Chemical Engineering, Chalmers University of Technology, Kemivägen 4,412 96, Gothenburg, Sweden*<br>*Department of Chemistry and Molecular Biology, Kemivägen 10, 412 96, Gothenburg, Sweden* | **Auditorium 2**<br>Session: **Thin films**<br>CHAIR: Dr. Igor Bdikin<br>***Keynote talk***<br>Dr. Joana Catarina Mendes **(I16)**<br>**Use of CVD Diamond films to improve the thermal management of GaN high electron mobility transistors: an historical overview**<br>*Instituto de Telecomunicações e Departamento de Eletrónica, Telecomunicações e Informática, Universidade de Aveiro, Portugal* |

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|---|---|---|
| 16:40-17:10 | Session: **Hydrogen and Fuel Cell Science**<br>***Keynote talk***<br>Dr. D. Pukazhselvan **(I21)**<br>**Consequence of graphene oxide to reduced graphene oxide transformation on the hydrogen storage behavior of GO/MgH2 composite**<br>*TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, 3810-193, Portugal* | Session: **Thin films**<br>***Keynote talk***<br>Dr. Venkata Eskilla Ramana **(I8)**<br>**Growth and ferroic physical properties of bismuth-layered magnetoelectric oxide thin films for low-loss energy-storage**<br>*3N-Aveiro, Department of Physics, University of Aveiro, Portugal* |
| 17:10-17:40 | Session: **Nanotechnology**<br>***Keynote talk***<br>Prof. Dr. Caue A. Martins **(I10)**<br>**Electrochemical conversion of glycerol into energy and carbonyl compounds using microfluidic systems**<br>*Institute of Physics, Federal University of Mato Grosso do Sul, Brazil* | Session: **Thin films**<br>Dr. Vahideh B. Isfahani **(O38)**<br>**Physical and electrochromic properties of Prussian Blue thin films prepared under different electrodeposion times on ITO substrates**<br>*Department of Physics & CICECO-Aveiro Institute of Materials, University of Aveiro, Aveiro-3810-193, Portugal* |
| 17:40-18:00 | Session: **Nanotechnology, Micro / Nano Materials**<br>Ms. Khadija EL KALAAOUI **(O15)**<br>**Zinc migration and its effect on the functionality of electrospun PVDF antibacterial nanofilms incorporated with ZnO nanoparticles**<br>*Laboratory LIMAT, Hassan II University of Casablanca, B.P 7955, Casablanca, Morocco* | Session: **Thin Films**<br>Mr. LABLALI Mohammed **(O12)**<br>**The growth of Cu thin film on stepped Si (001) substrates: Molecular dynamics study**<br>*Laboratory of Condensed Matter, Faculty of Science Ben M'Sick, University Hassan II of Casablanca, Morocco* |
| 18:00-18:20 | Session: **New Materials and Advanced Materials**<br>Ms. Vanessa Graça **(O33)**<br>**Ba2NiMoO6-δ as a potential electrode for protonic ceramic fuel cells at intermediate temperature (400-600°C)**<br>*Centre for Mechanical Technology and Automation, Mechanical Engineering Department, University of Aveiro, Aveiro, 3810-193, Portugal* | Session: **Low Dimension Structures**<br>Ms. Wafaa Salhi **(O20)**<br>**Double two-photon absorption in a asymmetric stepped quantum well in the terahertz range**<br>*Salhi Wafaa, Cadi Ayyad university, Marrakech, Morocco* |
| 18:20-18:40 | | Session: **Tribology in Manufacturing Processes**<br>Dr. Musa DEMİRCİ **(O25)**<br>**Wear Resistance of Recycled Polyamide Powder PA 3200 GF Produced by SLS**<br>*KTO Karatay University, Faculty of Engineering and Natural Sciences, Mechanical Engineering Department, Konya, Türkiye* |

# July 7, 2022 (Thursday)

## 5th International Conference on Nanomaterials Science and Mechanical Engineering (5th ICNMSME-2022) (*online*)

| | | |
|---|---|---|
| 9:00-10:00 | **Auditorium 1**<br>Session: **Micro / Nano Materials**<br>CHAIRS: Dr. Indrani Coondoo, Prof. Dr. Ezddin Hutli<br>***Plenary Lecture***<br>Prof. Dr. Marc Georg Willinger<br>**Novel applications of in-situ scanning electron microscopy in material science**<br>*Chair of Electron Microscopy with research emphasis on Energy Materials, Faculty of Chemistry, Technical University of Munich, Lichtenbergstraße 4, D-85748 Garching, Germany* | |
| 10:00-10:10 | Coffee break | |
| 10:10-10:40 | **Auditorium 1**<br>Session: **Optical Materials**<br>CHAIR: Dr. Indrani Coondoo<br>***Keynote talk***<br>Dr. Suresh Kumar Jakka **(I6)**<br>**Photoluminescence behaviour of Ho3+ with Yb3+ sensitizers in YOF nanocrystals**<br>*i3N, Department of Physics, University of Aveiro, Aveiro, Portugal* | **Auditorium2**<br>Session: **Biomaterials**<br>CHAIR: Prof. Dr. Ezddin Hutli<br>***Keynote talk***<br>Dr. Svitlana Kopyl **(I4)**<br>**Self-assembled Peptide Nanotubes of Different Chirality: Properties and Applications**<br>*Department of Physics & CICECO-Aveiro Institute of Materials, University of Aveiro, Portugal* |
| 10:40-11:10 | Session: **Composites/biomaterials**<br>Dr. Alaa Almansoori **(O36)**<br>**Novel application of plasma treatment of polymer and composite powders for 3D additive manufacturing**<br>*Technical Institute of Basra, Southern Technical University, Iraq* | Session: **Biomaterials**<br>***Keynote talk***<br>Dr. Vikram Pandit **(I9)**<br>**Development of Hydrogen production reactor system utilizing Water & Zinc Indium Sulfide**<br>*Haribhai V. Desai Arts, Science & Commerce College, Pune-411002, India* |

| | **Auditorium 1** Session: **Ceramics** | **Auditorium2** Session: **Biomaterials** |
|---|---|---|
| 11:10-11:40 | ***Keynote talk***<br>Prof. Dr. Andrei Kovalevsky **(I2)**<br>**Exploring the strategies towards enhancing the thermoelectric performance in oxide materials**<br>*CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal* | ***Keynote talk***<br>Dr. Ana Domínguez Bajo **(I19)**<br>**Reduced graphene oxide biomaterials as a potential therapy for spinal cord injury repair**<br>*Louvain Institute of Biomolecular Science and Technology (IBST). Croix du sud 4-5/L7.07.10. 1348 Louvain-la-Neuve, Belgium* |
| 11:40-12:10 | Session: **Micro / Nano Materials**<br>***Keynote talk***<br>Prof. Dr. Jamal Davoodi **(I13)**<br>**The comparative study of mechanical properties of armchair and zigzag borophene nanotubes**<br>*University of Zanjan, Zanjan, Iran* | Session: **Biomaterials**<br>Mr. Omkar Malusare **(O40)**<br>**Driving the photocatalytic activity of Fe2O3 towards TiO2 for Safranin & Rhodamine dye degradation**<br>*Haribhai V. Desai Arts, Science & Commerce College, Pune-411002, India* |
| 12:10-12:35 | Session: **Micro / Nano Materials**<br>***Keynote talk***<br>Prof. Dr. Radheshyam Rai **(I1)**<br>**Fabrication and charge transport study in Perovskite solar cell**<br>*School of Physics and Materials Science, Shoolini University, Solan, Himachal Pradesh 173229, India* | Session: **Biomaterials**<br>Mr. Sagar Mahajan **(O41)**<br>**Novel AgFe2O3-PQ Composite for the Photocatalytic Application**<br>*Haribhai V. Desai Arts, Science & Commerce College, Pune-411002, India* |
| 12:35-13:00 | Session: **Materials Sciences: Building materials**<br>***Keynote talk***<br>Dr. Elena Mercedes Perez Monserrat **(I14)**<br>**Firing and post-firing processes of historic Mg-rich calcareous bricks: high durability in very humid environments**<br>*Department of Geosciences, University of Padua, Via G. Gradenigo 6, 35131 Padua, Italy* | Session: **Biomaterials**<br>Ms. Zinaida Shakel **(O34)**<br>**Hyaluronic acid packed in transethosomes for topical delivery**<br>*LAQV, REQUIMTE, Department of Chemistry, Faculty of Pharmacy, University of Porto, Portugal* |
| 13:00-14:00 | Lunch | |

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| 14:00-14:50 | **Auditorium 1**<br>Session: **Sensor Materials**<br>CHAIRS: Dr. D. Pukazhselvan, Dr. Francisco Loureiro<br>***Plenary Lecture***<br>Prof. Dr. Pedro Alpuim<br>**Graphene micro and macro electronic sensing devices**<br>*International Iberian Nanotechnology Laboratory, Av. Mestre José Veiga s/n, Braga, Portugal*<br>*Centro de Física das Universidades do Minho e Porto, Universidade do Minho, Braga, Portugal* | |
| 14:50-15:40 | Session: **New Materials and Advanced Materials**<br>CHAIRS: Dr. D. Pukazhselvan, Dr. Francisco Loureiro<br>***Plenary Lecture***<br>Prof. Dr. Ezddin Hutli<br>**Thermal-Hydraulics Analysis of Light Water Reactors (BWR&PWR) and a High-Temperature-Gas Helium -Cooled Fast Breeder Reactor (GHFBR)**<br>*Centre for Energy Research, Budapest, Hungary*<br>*Institute of Nuclear Techniques, Budapest University of Technology and Economics, Budapest, Hungary* | |
| 15:40-15:50 | Coffee break | |
| 15:50-16:20 | **Auditorium 1**<br>Session: **Nanotechnology**<br>CHAIR: Dr. D. Pukazhselvan<br>***Keynote talk***<br>Prof. Dr. Thangaraju Dheivasigamani **(I17)**<br>**High temperature wet chemical synthesis of two dimensional chalcogenide nanosheets for photodetector applications**<br>*nano-crystal Design and Application Lab (n-DAL), Department of Physics, PSG Institute of Technology and Applied Research, Coimbatore-641062, Tamil Nadu, India* | **Auditorium 2**<br>Session: **Ceramics**<br>CHAIR: Dr. Francisco Loureiro, Dr. Igor Bdikin<br>***Keynote talk***<br>Dr. S. Shanmuga Sundari **(I7)**<br>**Impact of Li+ ion irradiation on structural, optical, electrical and morphological properties of BaSnO3 ceramics**<br>*Department of Physics, PSGR Krishnammal College for Women, Coimbatore, 641004, India* |

<table>
<tr><td>16:20-<br>16:50</td><td>Session: New Energy Materials<br>Keynote talk<br><br>Prof. Dr. Heberton Wender (I11)<br>Basic principles and recent advances of photocatalytic fuel cells<br>Institute of Physics – Federal University of Mato Grosso do Sul, Brazil</td><td>Session: 2D materials<br><br>Mr. Ganesh Jadhav (O39)<br>Water Pollution control & Hydrogen Production using 2D- Photocatalyst: 6, 13-Pentacenequinone (PQ)<br>Haribhai V. Desai Arts, Science & Commerce College, Pune-411002, India</td></tr>
<tr><td>16:50-<br>17:00</td><td colspan="2">Coffee break</td></tr>
<tr><td rowspan="2">17:00-<br>18:30</td><td colspan="2">Evening Poster Sessions</td></tr>
<tr><td>Auditorium 1<br><br>CHAIR: Dr. D. Pukazhselvan<br><br>P1-P12</td><td>Auditorium 2<br><br>CHAIR: Dr. Francisco Loureiro, Dr. Igor Bdikin<br><br>P13-P25</td></tr>
</table>

# July 8, 2022 (Friday)

## 5th International Conference on Nanomaterials Science and Mechanical Engineering (5th ICNMSME-2022) (online)

<table>
<tr><td>9:00-<br>9:30</td><td colspan="2">Auditorium 1<br><br>Session: Company presentations<br>CHAIRS: Dr. Pukazh Selvan Dharmakkon,<br>Dr. Gil Gonçalves<br><br>Dr. Nicolas F. Martinez (C1)<br>Advanced nano-electrical characterization of solar cells and 2-D materials with Atomic Force Microcopy<br>Concept Scientific Instruments, 2 Rue de la Terre de Feu, 91940 Les Ulis, France</td></tr>
<tr><td>9:30-<br>10:00</td><td colspan="2">Session: New Materials and Advanced Materials<br>CHAIRS: Dr. Pukazh Selvan Dharmakkon,<br>Dr. Gil Gonçalves<br><br>Plenary Lecture<br><br>Prof. Dr. Yuri Dekhtyar<br>Kinetics of strength via electron emission of composite nanolayer<br>Riga Technical University, Kipsalas 6A, Riga, Latvia LV1048</td></tr>
<tr><td>10:00-<br>10:10</td><td colspan="2">Coffee break</td></tr>
<tr><td>10:10-<br>10:25</td><td>Auditorium 1<br><br>Session: Micro / Nano Materials<br>CHAIR: Dr. Pukazh Selvan Dharmakkon<br><br>Prof. Dr. Lynda Djoudi (O23)<br>Synthesis and structural Characterization of Cu Substituted SrCoO3 Perovskite Oxides<br>Laboratory of Molecular Chemistry and Environment, University Mohamed Khider of Biskra, 07000 - Algeria</td><td>Auditorium 2<br><br>Session: Engineering & Technology<br>CHAIR: Dr. Gil Gonçalves<br><br>Mr. Miguel Montenegro (O17)<br>Rheological characterization of eco-friendly non-Brownian suspensions<br>Transport Phenomena Research Center (CEFT), Mechanical Engineering Department, Faculty of Engineering of the University of Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal</td></tr>
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| 10:25-10:40 | Session: **New Energy Materials, Nanotechnology**<br><br>Dr. Serbülent Türk **(O8)**<br>**A novel conductive PEDOT:PSS/GG hydrogel electrolyte based dye sensitized solar cell**<br>*Sakarya University, Biomedical, Magnetic and Semiconductor Materials Application and Research Center (BIMAS-RC), 54187 Sakarya, Turkey* | Session: **Mechanics & Materials**<br><br>Mr. Fettah Bilal **(O6)**<br>**Experimental Evaluation of Metal foam for design as a bearing Damper Replaced Old Squeeze Film Damper**<br>*Laboratory of Rheology and Mechanics, Hassiba Benbouali University of Chlef, Algeria* |
| 10:40-11:00 | Session: **New Energy Materials**<br><br>Dr. Francisco Loureiro **(O3)**<br>**Lithium titanium phosphate materials for Li-ion batteries: study of the grain boundary properties with boron addition**<br>*Centre for Mechanical Technology and Automation, Mechanical Engineering Department, University of Aveiro, Aveiro, 3810-193, Portugal* | Session: **Tribology in Manufacturing Processes**<br><br>Dr. Musa DEMİRCİ **(O25)**<br>**Wear Resistance of Recycled Polyamide Powder PA 3200 GF Produced by SLS**<br>*KTO Karatay University, Faculty of Engineering and Natural Sciences, Mechanical Engineering Department, Konya, Türkiye*<br>*(New time for this presentation: July 6, 2022 (Wednesday, 18:20-18:40))* |
| 11:00-11:20 | Session: **New Energy Materials**<br><br>Mr. Diogo Lopes **(O28)**<br>**SrTiO3-based thermoelectric fibres grown using Laser Floating Zone processing**<br>*CICECO–Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal* | Session: **New Methods of Modeling Properties Materials**<br><br>Mr. Rajat Verma (O10)<br>**Performance Analysis for the Improvement of Worn Hydrodynamic Journal Bearings with Nano-Fluids used in Heavy Industrial Machinery : A Numerical Simulation Approach**<br>*SMVDU Katra, J&K, India* |
| 11:20-11:35 | Session: **Hydrogen and fuel cell science**<br><br>Ms. Laura Holz **(O27)**<br>**Vanadium (oxy)nitride as a potential anode for ammonia solid oxide fuel cells**<br>*Centre for Mechanical Technology and Automation, Mechanical Engineering Department, University of Aveiro, Aveiro, 3810-193, Portugal* | Session: **Environmental Fluid Mechanics**<br><br>Dr. Lamia Ben Ramoul **(O11)**<br>**Effect of the orientation of urban streets canyon compared to the principal axis of wind on the dispersion of pollutants in the cities**<br>*Laboratory of Mechanics, Physics and Mathematical Modeling, University of Medea, Algeria* |
| 11:35-11:40 | Coffee break | |

| | **Auditorium 1** | **Auditorium 2** |
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| | Session: **Nanotechnology, Micro / Nano Materials**<br>CHAIR: Dr. Pukazh Selvan Dharmakkon | Session: **Engineering & Technology**<br>CHAIR: Gil Gonçalves |
| 11:40-11:55 | Ms. Oumaima BILI **(O14)**<br>**Flame retardant and hydrophobic PVDF/[Imim][PF6] membranes elaborated by electrospinning method**<br>*Laboratory LIMAT, Hassan II University of Casablanca, B.P 7955, Casablanca, Morocco* | Mr. Pedro C. Rijo **(O16)**<br>**Rheological Characterization of 2D Nanoparticles Suspensions**<br>*Transport Phenomena Research Center (CEFT), Mechanical Department, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal* |
| | Session: **Micro / Nano Materials** | Session: **Thermal Engineering Theory and Applications** |
| 11:55-12:10 | Ms. Dimitra Das **(O5)**<br>**Photocatalytic degradation of toxic pollutants from waste-water by thermally-modified Graphitic Carbon Nitride**<br>*School of Materials Science and Nanotechnology, Jadavpur University, 188, Raja S.C. Mallick Road, Kolkata- 700032, India* | Ms. Cheriet Nacera **(O9)**<br>**Passive methods in heat transfer enhancement over heated blocks using airfoil generator**<br>*Laboratory of Mechanics, Physics and Mathematical Modeling (LMP2M), Medea, Algeria* |
| | Session: **New Materials and Advanced Materials** | Session: **Thermal Engineering Theory and Applications** |
| 12:10-12:25 | Ms. EL OTMANI RKIA **(O13)**<br>**Electrodeposition of manganese sulphide (MnS) thin films : characterization and chelating agents effect**<br>*MED-Lab, Université Cadi Ayyad, Faculté des Sciences et Techniques, BP 549, 40000 Marrakech, Morocco* | Mr. Ahmed El Hamdaoui **(O21)**<br>**Computational insight into thermal and vibrational properties of the fresnoite and the barium titanosilicate glasses**<br>*University Hassan II, Casablanca, Morocco* |
| | Session: **Micro / Nano Materials** | Session: **Engineering Optimization** |
| 12:25-12:45 | Prof. Dr. Andrzej Kudelski **(O4)**<br>**New Plasmonic-Magnetic Nanomaterials for Shell-Isolated Nanoparticle-Enhanced Raman Spectroscopy (SHINERS)**<br>*Faculty of Chemistry, University of Warsaw, ul. Pasteura 1, 02-093 Warsaw, Poland* | Mr. Abdellatif Elaakili **(O19)**<br>**The application of different orientation of orthotropic composite beam**<br>*Mohammed V University in Rabat, Morocco* |

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| | Session: **Micro / Nano Materials** | Session: **Composite, Building Materials** |
| 12:45-13:00 | Ms. Justyna Niewiadomska-Kaplar **(O2)**<br>**New approach to the molecular electronics of fluorographene**<br>*Scientific Publishing House Tab, Rome, Italy* | Mr. Moad NADI **(O22)**<br>**Effect of natural graphite addition on metakaolin based geopolymers: A Mechanical and Microstructural Study**<br>*Laboratory of engineering and materials LIMAT, Faculty of Science Ben M'Sik, Hassan II University, Casablanca, Morocco* |
| 13:00-14:00 | Lunch | |
| | **Auditorium 1**<br>Session: **Materials Science: Metal alloy Materials**<br>CHAIR: Dr. Duncan Fagg, Dr. Igor Bdikin | **Auditorium 2**<br>Session: **Optical Materials**<br>CHAIR: Dr. Suresh Kumar Jakka |
| 14:00-14:20 | Ms. Daniela V. Lopes **(O26)**<br>**Exploring the Ti influence on the electrochemical reduction of iron from iron oxide based ceramics**<br>*CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal* | Ms. Ramadevi Suguru Pathinti **(O43)**<br>**Electro – Optical Performance of Coumarin dye doped Cholesteric liquid crystals for the Application of Electrically Switchable Smart Window**<br>*Department of Physics, National Institute of Technology, Warangal, Telangana, India* |
| | Session: **Materials Science: Metal alloy Materials** | Session: **Sensor Materials** |
| 14:20-14:40 | Mr. Francisco H. Duarte **(O31)**<br>**Prospects of iron electrowinning from an iron-rich industrial residue**<br>*CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal* | Mr. Buchaiah Gollapelli (O32)<br>**Detection of Bile acids using Optical Biosensors based on Cholesteric Liquid Crystal Droplets**<br>*Department of Physics, National Institute of Technology, Warangal 506004, INDIA* |

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| 14:40-15:10 | Session: **Thin films**<br>***Keynote talk***<br>Prof. Dr. V. R. Singh **(I12)**<br>**Electronic and Magnetic Properties of Diluted Magnetic Semiconductor Thin Films: A Synchrotron based X-Ray Spectroscopic Techniques**<br>*Department of Physics, Central University of South Bihar, Gaya, India* | Session: **Optical thermal sensors**<br>***Keynote talk***<br>Prof. Dr. Pavani Krishnapuram **(I20)**<br>**Diverse Optical thermal sensing mechanisms in rare earth activated Aurivilliu's family compound**<br>*I3N-Department of Physics, University of Aveiro, Aveiro, Portugal* |
| 15:10-15:20 | Coffee break | |
| 15:20-15:50 | Session: **New Materials and Advanced Materials**<br>CHAIR: Dr. Duncan Fagg<br>***Keynote talk***<br>Dr. Pavel Zelenovskii **(I18)**<br>**Role of the molecule's conformation on the piezoelectric properties of diphenylalanine nanostructures**<br>*Department of Chemistry & CICECO–Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal* | Session: **Micro / Nano Materials**<br>CHAIR: Dr. Suresh Kumar Jakka<br>***Keynote talk***<br>Dr. Indrani Coondoo **(I5)**<br>**Magnetoelectric coupling studies in lead-free multiferroic ceramic composites**<br>*Department of Physics & CICECO, University of Aveiro, Portugal* |
| 15:50-16:10 | Session: **Materials Science: Metal alloy Materials**<br>Dr. Aleksey Lisenkov **(O30)**<br>**Impact of the substrate composition to the deposition process of the iron from highly alkaline suspensions**<br>*Department of Materials and Ceramic Engineering/ CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193, Aveiro, Portugal* | Session: **Sensor Materials**<br>Ms. Salma Moussadeq **(O24)**<br>**The study of Benzene adsorption on clean and doped Ag (100) surfaces using DFT**<br>*Laboratoire de physique de la matière condensée (LPMC), Faculté des sciences BEN M'SIK, Université HASSAN II de CASABLANCA, MAROC* |

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| 16:10-16:30 | Session: **Ceramics**<br><br>Ms. Parisa Amirkhizi **(O29)**<br>**Tunning the Thermoelectric properties via Substitution and Defect Chemistry engineering by Taguchi plan**<br>*Department of Materials and Ceramics Engineering, CICECO-Aveiro Institute of Materials, University of Aveiro, Aveiro, 3810-193, Portugal* | Session: **Micro / Nano Materials**<br><br>Dr. Nandipha L. Botha **(O1)**<br>**Green synthesis of metal sulphide nanoparticles: Morphological, chemical, optical properties and activity as nanofertilizers**<br>*UNESCO-UNISA Africa Chair in Nanosciences-Nanotechnology, College of Graduate Studies, Muckleneuk ridge, Pretoria, South Africa* |
| 16:30-16:50 | Session: **Biomaterials**<br><br>***Keynote talk***<br><br>Prof. Dr. Maciej Wojtaś **(I15)**<br>**New piezoelectric in Pirydyl-Alanine based hybrid crystal**<br>*Faculty of Chemistry, University of Wrocław, 14 Joliot-Curie, 50-383 Wrocław, Poland* | Session: **Micro / Nano Materials**<br><br>Ms. Gamze Ozcakir **(O35)**<br>**Synthesis of ambient pressure–dried hydrophobic silica aerogel**<br>*Chemical Engineering Department, Faculty of Engineering, Bilecik Seyh Edebali University, Gulumbe Campus, 11210, Bilecik, Turkey* |
| 16:50-17:10 | Session: **Biomaterials**<br><br>Mr. Youssef Ouldhnini **(O18)**<br>**Insights on the Structural Properties of 45S5 Bioactive Nanoglasses via Molecular dynamics Simulations**<br>*LS2ME, Faculté Polydisciplinaire Khouribga, Sultan Moulay Slimane University of Beni Mellal, B.P 145, 25000 Khouribga, Morocco* | Session: **Ceramics**<br><br>Mr. Milan Vukšić **(O37)**<br>**Solid waste recycling in alumina technical ceramics production**<br>*Department of Materials, Faculty of Mechanical Engineering and Naval Architecture University of Zagreb, Ivana Lučića 1, 10000 Zagreb, Croatia* |
| 17:10-17:30 | Session: **Environmental Friendly Materials**<br><br>Prof. Dr. Francisco Jesús Fernández-Morales (O42)<br>**Effect of HTC doping on the performance of carbon felt as anodic electrode in microbial fuel cells**<br>*Department of Chemical Engineering, Faculty of Chemical Sciences and Technologies, University of Castilla La Mancha, Spain* | Session: **Protective Coatings and Corrosion of Materials**<br><br>Ms. Amira Gharbi **(O7)**<br>**Corrosion Inhibition using ethanolic extract of a Ficus elastica in 1M HCL**<br>*Process Engineering Department, University of Souk Ahras, 41000, Algeria* |
| 17:30-18:00 | **Auditorium 1**<br><br>**Conference Closing Ceremony** | |

# Poster session, July 7, 2022 (Thursday), 17:00-18:30

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| **P1** | **Conductivity and transmittance enhancement of PEDOT:PSS thin films by graphene addition**<br>Mabilia, Felipe Teixeira, Wang, Shu Hui<br>*Universidade de São Paulo, Escola Politécnica, Departamento de Engenharia Metalúrgica e de Materiais, Av. Professor Mello Moraes, 2463, CEP: 05508-030, São Paulo/SP, Brazil* |
| **P2** | **Synthesis and characterization of ZnAl new hybrid layered double hydroxide. Application to uranyl adsorption**<br>Kenza Drissi, Hajer Azzi,M'hamed Kaid , Didier Villemin<br>*University of Ain Temouchent, Faculty of Sciences and Technology, BP 284,46000 Ain Temouchent, Algeria; Laboratory of Catalysis and Synthesis in Organic Chemistry LCSCO – University of Tlemcen. Tlemcen.Algeria; Laboratory of physico-chimical research, Departement of Chemistry, Faculty of Sciences . University Dr Moulay Taher. BP 138 Ennasr. Saida. Algeria; LCMT, EnsiCaen, , UMR CNRS 6507, Caen, France* |
| **P3** | **Lithium titanium phosphate materials for Li-ion batteries: study of the grain boundary properties with boron addition**<br>Francisco J. A. Loureiro, Zinaida Shakel, Bruno M. G. Melo, Vanessa C. D. Graça, Laura I. V. Holz, Sergey M. Mikhalev, Aliaksandr L. Shaula, Duncan P. Fagg<br>*Centre for Mechanical Technology and Automation, Mechanical Engineering Department, University of Aveiro, Aveiro, 3810-193, Portugal; I3N, Department of Physics, University of Aveiro, Aveiro 3810-193, Portugal* |
| **P4** | **Degradation of azo-dye by Fenton and photo-Fenton using surface-functionalized polyacrylonitrile (PAN) fibre catalyst**<br>Martina Kocijan, Sanaa Rashid, Katherine Huddersman<br>*Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Ivana Lučića 5, 10000 Zagreb, Croatia; Faculty of Health and Life Sciences, De Montfort University, The Gateway, Leicester LE1 9BH, UK* |
| **P5** | **Correlations among mechanical properties of camel hair fiber and polypropylene fiber reinforced concrete at high temperature**<br>ILhem Sahnoun, Hocine CHabil , TOUMI BELKACEM<br>*Materials and Sustainability Laboratory (LMDC), Route Ain El bey, Constantine, Algeria* |
| **P6** | **Numerical investigation of Mixed convective heat transfer in a channel in presence baffles**<br>Toumi Hayet, Rabah Henniche<br>*Laboratory of Mechanics, Physics and Mathematical Modeling (LMP2M), Medea, Algeria* |

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| **P7** | **Impact of Transition of Metal oxides (TiO2, MnO, CuO) On Structural, and Optical properties of Core Shell heterostructure CdS/Zn3(PO4)2 Nanohybrid for LED applications**<br>G. Sreedevi, S.K. Jakka, K. Pavani, V.Jayalakshmi, K.Venkatarao, Sandhya Cole<br>*Dept.of Physics, PVP Siddhartha Institute of Technology, Vijayawada, A.P., India; I3N & Department of Physics, University of Aveiro, Aveiro 3810-193, Portugal; Dept.of Physics, National Institute of Technology, Warangal,Telangana., India; Dept.of Physics, Government Polytechnic, Krosuru, Guntur, A.P., India; Dept.of Physics, Acharya Nagarjuna University, Nagarjuna Nagar, A.P., India* |
| **P8** | **Mechanical Properties of pristine and carbon nanotube poly (2, 5-benzimidazole) composite: A molecular dynamics and experimental approach**<br>Lynndle Square, Lionel Fourie<br>*Centre for Space Research, North-West University, Potchefstroom, South Africa; Department of Physics and Astronomy, University of the Western Cape, Bellville, South Africa* |
| **P9** | **Novel hybrid nanofibrous membranes of Nylon 6/Yeast cell wall components for potential removal of heavy metal contaminants**<br>Rodolfo Ferreira, Rodrigo Colhe, Elisabete Coelho, José A. Lopes da Silva<br>*LAQV-REQUIMTE and Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal* |
| **P10** | **Corrosion protection of pipeline steels by organic inhibitors**<br>Nadjette Belhamra, Fatima Benmessoud, Maria N. Boumerzak<br>*Physic Laboratory of Thin Films and Applications (LPCMA), University of Biskra, 07000, Algeria* |
| **P11** | **Ultra-small iron oxide nanoparticles synthesized by gamma irradiation**<br>Zorai Amel, Abdelhafid Souici, Salim Ouhenia, Jacqueline Belloni, Mehran Mostafavi and Eric Rivière<br>*Laboratory of Physical Chemistry of Materials and Catalysis (LPCMC), Group of Crystallography and Materials Simulation. Faculty of Exact Sciences, University of Bejaia, CP 06000 Bejaia, Algeria; Institut de Chimie Physique (ICP), UMR-8000, CNRS-UPS, Université Paris-Saclay, 15 Avenue Jean Perrin, Bâtiment 349, 91405 Orsay, France; Institut de Chimie Moléculaire et des Matériaux d'Orsay (ICMMO), Université Paris-Saclay, CNRS, 410 Rue du Doyen Georges Poitou, 91405 Orsay, France* |
| **P12** | **Mechanical spectroscopy of SiO2/Si, nanocomposites of multiwalled carbon nanotubes and polyamide, polyvinyl chloride, polyethylene, porous polystyrene**<br>A.P. Onanko, D.V. Charnyi, M.V. Yatsiuk, Y.A. Onanko, O.P. Dmytrenko, M.P. Kulish, T.M. Pinchuk-Rugal, O.L. Pavlenko, T.O. Busko, A.A. Kuzmych, P.P. Ilyin<br>*Kyiv national university, Kyiv, Ukraine* |
| **P13** | **Optical and Morphological properties of Nb2O5 thin films grown by HiPIMS at room temperature**<br>L. P. G Oliveira, R. Ramos, E. Martins, E. C. Rangel, S. F. Durrant, N. C. Cruz and J. R. R. Bortoleto<br>*São Paulo State University (UNESP), Av. 3 de Março 511, Sorocaba, SP, Brazil* |

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| **P14** | **Development of magnetic PLA/CaP composites**<br>T.S.S. Carvalho, N. Ribeiro, P.M.C. Torres, J.C. Almeida, J.H. Belo, J. P. Araújo, A. Ramos, M. Oliveira and S.M. Olhero<br>*Department of Materials Engineering and Ceramics (DEMaC), CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193, Aveiro, Portugal; Departament of Mechanical Engineering, TEMA-Centre for Mechanical Technology and Automation, University of Aveiro, Portugal; i3S – Instituto de Investigação e Inovação em Saúde, Universidade do Porto, Porto, Portugal; INEB – Instituto Nacional de Engenharia Biomédica, 4200-135, Portugal; Institute of Physics of Advanced Materials, Nanotechnology and Photonics (IFIMUP), Department of Physics and Astronomy, University of Porto, 4169-007 Porto, Portugal* |
| **P15** | **Novel thermoelectric composites based on n-type SrTiO3 for high-temperature energy harvesting**<br>Tiago Paulino, Wenjie Xie, Anke Weidenkaff, Andrei Kovalevsky, Gabriel Constantinescu<br>*Department of Materials and Ceramic Engineering, CICECO—Aveiro Institute of Materials, University of Aveiro, Aveiro, 3810-193, Portugal; Institute of Materials Science, Technische Universitat Darmstadt, Alarich-Weiss-Str. 2, Darmstadt, 64287, Germany; Fraunhofer Research Institution for Materials Recycling and Resource Strategies IWKS, Brentanostraße 2a, Alzenau, 63755, Germany* |
| **P16** | **Agarose hydrogels modified by silk fibroin as materials with tunable transport and rheological properties**<br>Veronika Richterová, Miloslav Pekař<br>*Faculty of Chemistry, Brno University of Technology, Purkyňova 464/118, 612 00 Brno, Czech Republic* |
| **P17** | **Synthesis of Zeolite H-ZSM-5 for Fischer Tropsch synthesis**<br>Saureille Ngouana Moafor, John Ngolui Lambi, Linda L. Jewell<br>*Laboratory of Material Chemistry, Department of Inorganic Chemistry, University of Yaounde I, P.O.BOX 812, Yaounde, Cameroon; Department of Chemical Engineering, University of South Africa (UNISA), Christiaan De Wet & Pioneer Avenue, Florida, 1710, South Africa* |
| **P18** | **Cytocompatible gelatin/boronsilicate hybrid materials**<br>J.C. Almeida, T.R. Correia, P.M.C. Torres, S.M. Olhero, A. Ramos<br>*Departament of Materials Engineering and Ceramics, CICECO-Aveiro Institute of Materials, University of Aveiro, Portugal; Departament of Chemistry, CICECO-Aveiro Institute of Materials, University of Aveiro, Portugal; Departament of Mechanical Engineering, TEMA-Centre for Mechanical Technology and Automation, University of Aveiro, Portugal* |
| **P19** | **Advantages of using sequential chemical fractionation to alkaline extraction for accessing the organic matter in biochar**<br>David Širůček, Michal Kalina, Martina Klučáková<br>*Faculty of Chemistry, Brno University of Technology, Purkyňova 464/118, 612 00 Brno, Czech Republic* |

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| **P20** | **Hydrogenated amorphous carbon-based coatings for orthodontics: bacterial adhesion**<br>António Fróis, Emanuel Cardoso, Luís F. Santos, Paula V. Morais, Romeu Francisco, and Cristina S. Louro<br>*CEMMPRE, Department of Mechanical Engineering, Faculty of Sciences and Technology, University of Coimbra, Rua Luis Reis Santos, 3030-177 Coimbra, Portugal; Biophysics Institute, Faculty of Medicine, University of Coimbra; Coimbra Institute for Clinical and Biomedical Research/Centre for Innovative Biomedicine and Biotechnology (iCBR/CIBB), 3000- 548 Coimbra, Portugal; CEMMPRE, Department of Life Sciences, Faculty of Sciences and Technology, University of Coimbra, Calçada Martim de Freitas, 3000-456 Coimbra, Portugal; Centro de Química Estrutural, Institute of Molecular Sciences and Dept. de Engenharia Química; IST, University of Lisbon, Av. Rovisco Pais, 1049-001 Lisboa, Portugal* |
| **P21** | **Synthesis, Characterization of Three Distinct Phases of Bismuth Molybdate for Supercapacitor Applications**<br>S. Bagavathy, D. Thangaraju, A. Durairajan, M.A. Valente<br>*nano-crystal Design and Application Lab (n-DAL), Department of Physics, PSG Institute of Technology and Applied Research, Coimbatore-641062, Tamil Nadu, India; I3N Aveiro, Department of Physics, University of Aveiro, 3810 193 Aveiro, Portugal* |
| **P22** | **Synthesis and Characterization of pure β-Bi2Mo2O9 and Eu-doped β-Bi2Mo2O9 for Photocatalytic applications**<br>S. Priyadharshini, D. Thangaraju, A. Durairajan, M.A. Valente<br>*nano-crystal Design and Application Lab (n-DAL), Department of Physics, PSG Institute of Technology and Applied Research, Coimbatore-641062, Tamil Nadu, India; I3N Aveiro, Department of Physics, University of Aveiro, 3810 193 Aveiro, Portugal* |
| **P23** | **Development of 2D MoS2 nanosheets on Lotus fibres for enhanced Hydrophobicity and Anti-microbial activity**<br>S.S. Govarthini, D. Thangaraju, A. Durairajan, M.P.F. Graça<br>*nano-crystal Design and Application Lab (n-DAL), Department of Physics, PSG Institute of Technology and Applied Research, Coimbatore-641062, Tamil Nadu, India; I3N Aveiro, Department of Physics, University of Aveiro, 3810 193 Aveiro, Portugal* |
| **P24** | **Room temperature synthesis and characterization of ZIF-8**<br>Gamze Ozcakir, Caglayan Acikgoz<br>*Chemical Engineering Department, Faculty of Engineering, Bilecik Seyh Edebali University, Gulumbe Campus, 11210, Bilecik, Turkey; Chemical Engineering Department, Faculty of Engineering, Bilecik Seyh Edebali University, Gulumbe Campus, 11210, Bilecik, Turkey* |
| **P25** | **Plastic waste as optimum feedstock for CD-based anticounterfeit tracers**<br>Raul Simões, Gil Gonçalves, Teresa Monteiro and Victor Neto<br>*Department of Mechanical Engineering; Centre for Mechanical Technology and Automation; University of Aveiro, Portugal; i3N, Department of Physics, University of Aveiro, Portugal* |

# Plenary lectures

# Novel applications of in-situ scanning electron microscopy in material science

**Marc Willinger ***

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Scanning electron microscopes are very versatile analytical instruments that provide insight into morphology, topology, composition and structure of materials down to the nanometer level. Based on the works of Garry Danilatos [1], modifications of the vacuum system and specially designed detectors have opened up the ability to study materials not only in vacuum, but also under defined atmospheres. This has enabled observation of non-conducting or wet (organic) specimens, and even opened the door to real-time in-situ observation of gas-phase and temperature induced processes.

In my presentation, I will try to advertise in-situ SEM as very potential and versatile analytical method. It will be shown that the instrument is capable of atomic scale resolution in surface coverage. Taking the example of graphene growth by chemical vapor deposition inside the chamber of an environmental SEM [2], it will be shown that direct observation of graphene growth delivers insights that can be used, for example, for controlled growth of twisted layer graphene.

By combining complementary analytical tools with in-situ SEM, the instruments capabilities can be further expanded. Examples from combined AFM and SEM studies will be shown, as well as recent results on in-situ calorimetric measurements during phase transitions. Finally, one important application is the study on chemically induced processes. Here, possible applications range from corrosion of metals, to green steel making and observation of active catalysts [3].

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# Printable smart and multifunctional materials for a digital and sustainable transformation

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Smart and multifunctional materials are a key driving force for the development of wireless, sustainable and interconnected systems, playing a central role in the scope of the digitalization and circular economy paradigms. Active and multifunctional materials are being, in fact, increasingly implemented in areas such as sensors and actuators, energy generation and storage, among others. The successful development of applications relies both in the ability to proper tailor their functional response and in their application with suitable (and sustainable) fabrication technologies.

Polymer based multifunctional materials processable by additive manufacturing technologies is an area of increasing interest due to improved sustainability, simple integration into devices and the possibility of obtaining multifunctional materials over large and flexible areas.

Strategies and challenges in the development of active and multifunctional materials, including electro-, magneto-, thermos- and photoactive, will be presented and discussed, together with applications in the areas of sensors, actuators and energy generation and storage.

**Acknowledgements**

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# Kinetics of strength via electron emission of composite nanolayer

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A theory of strength kinetic nature was developed in the 70th of the XX century [1]. However, it was unknown, if the theory works at a nanoscale.

The report considers issues by the kinetic theory to be bridged with an electron emission from a nanolayer of a loading solid. When atomic/molecular couples situated at the nanolayer of the loading material are tensed or destructed. As a result electron density of states changes and electron emission has specificities.

Electron emission was detected in the near threshold mode. A carbon nanotube-reinforced epoxy composite (NREC) was chosen as an example.

It was observed that emission appeared at ~ 0.3 % of strain. This was considered as a message of earlier destruction. An emission current was delivered as stochastic pulses. Their appearing frequency was connected to the duration of loading. The discovered correlation of pulses frequency with mechanical strength evidenced that the nanolayer of the material destructed in accordance with the kinetic theory of strength.

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# Tunnel magnetoresistance in granular ferro(ferri)magnetic systems

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Tunnel magnetoresistance (TMR) occurs in a magnetic tunnel junction (MTJ) consisting of two ferro(ferri)magnetic (FM) electrodes separated by a thin insulator. Following the simple Julliére model [1], the FM electrodes should be selected with the highest possible spin polarization $P$ at room temperature. In this context, an analysis of its temperature dependence was made considering FM metals, manganites, double perovskites and magnetite. Intergranular magnetoresistance caused by spin-dependent tunneling is then determined by (i) the spin polarization and (ii) the reduced magnetization $m = M/M_S$ with $M_S$ the saturated magnetization.

First, we consider superparamagnetic granular systems. In this case, $m$ is described by the Langevin function including the magnetic moment $\mu$, the magnetic flux density $B$ and the temperature $T$ as parameters. The critical size below which superparamagnetic behavior is obtained, was estimated for ferromagnetic metals and strontium ferromolybdate (SFMO). The values $m(T)$ and $m(B)$ were evaluated for Fe in dependence on nanoparticle size as well as for SFMO. The resulting magnetic field sensibility of superparamagnetic sensors was far too low for practical application.

Up to now, there is no satisfactory analytical expression for $m(T)$ except two limiting cases: (i) near Curie temperature and (ii) at very low temperatures. Different available models were reviewed. In this work, an approximation of $m(T)^2$ derived for Ni near Curie temperature [2] was applied in a series expansion. The magnetic flux density dependence was modeled by means of a traditional analysis of the approach of magnetization to saturation [3]. The calculated maximum field sensitivity of granular MTJs amounted to 6.6%/T, 14.6%/T and 32%/T for SFMO, Co and Fe, respectively, i.e. one order of magnitude less than planar MTJs.

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# Catechol and its analogues in hydrogels and in electrodeposited films

**Vincent BALL** [1,2], Kevin Ziegler [1,4], Florence Back [1,2], Nataly Ortiz-Pena [3], Ovidiu Ersen [3], Tanja Weil [4], Clément Sanchez [5]

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Polyphenols are a broad class of molecules playing (often ignored) fondamental roles in biology: they contribute to the defense of plants against herbivores, they ensure the mechanical stability of wood and are often antioxidant and antibactericidal. They are also surface active and some of them deposit spontaneously at solid-liquid interfaces to form conformal films alone or in combination with metal cations with which they can form strong coordination complexes. In this presentation we will describe how the smallest polyphenol, 1,2-dihydydroxybenzene (catechol), its isomers and related molecules can be used as active components in hydrogels to increase their adhesion on steel [1] and can be electropolymerized on electrodes [2-4] to yield conformal films displaying some analogy with graphene oxide based films.

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# Thermal-Hydraulics Analysis of Light Water Reactors (BWR&PWR) and a High-Temperature-Gas Helium -Cooled Fast Breeder Reactor (GHFBR)

**Ezddin Hutli** [1,2]
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[2]*Institute of Nuclear Techniques, Budapest University of Technology and Economics, Budapest, Hungary*

The lecture focuses on thermal-hydraulic analysis, which is important in nuclear power system efficiency and choosing the optimal nuclear reactor design. At nominal operating conditions, a steady-state thermal-hydraulic analysis of the core of the Light Water Reactor (BWR&PWR) and a high-temperature helium-gas-cooled Fast Breeder reactor (GHFBR) will be presented. As test cases, a typical BWR/6 (GE model), a typical (Westinghouse model) Pressurized Water Reactor (PWR), and a typical Gas Heilum-Cooled Fast Breeder Reactor (GHFBR) were used. The goal of the analysis is to determine how to maintain the thermal safety margin and core integrity under steady-state operating conditions. The effect of operating conditions such as power distribution, power level, and coolant mass flow rate on the performance of the proposed core will be discussed. The one-dimensional computer codes MITH and MIGHT were used for this purpose. The reliability of each code was evaluated using the GE benchmark 3579 MWt reactor, the W- benchmark 3411 MWt (BWR and PWR, respectively), and the GCFBR benchmark 2530 MWt. Two-channel models were tested in all cases (the average and the hot channel). Along the tested channels, thermal-hydraulic parameters such as fuel-centerline, fuel-surface, outer clad surface, and coolant temperature, critical and actual local heat flux, Departure and Minimum Departure from Nucleate Boiling (DNBR and MDNBR, respectively), and pressure drop are calculated. Temperatures, as well as actual and critical heat flux distribution profiles, were obtained. The tested operating conditions had a significant impact on these parameters, as well as the thermal-hydraulic performance. The obtained results are in good agreement with the data from the tested cores. The obtained results are well within the safety margins. The good agreement between the tested reactor data and the applied codes calculation concerning the reactors demonstrates the reliability of the analysis methodology from a thermal-hydraulic point of view.

# The Computational Microscope: a Versatile Tool to Understand and Design NanoMaterials

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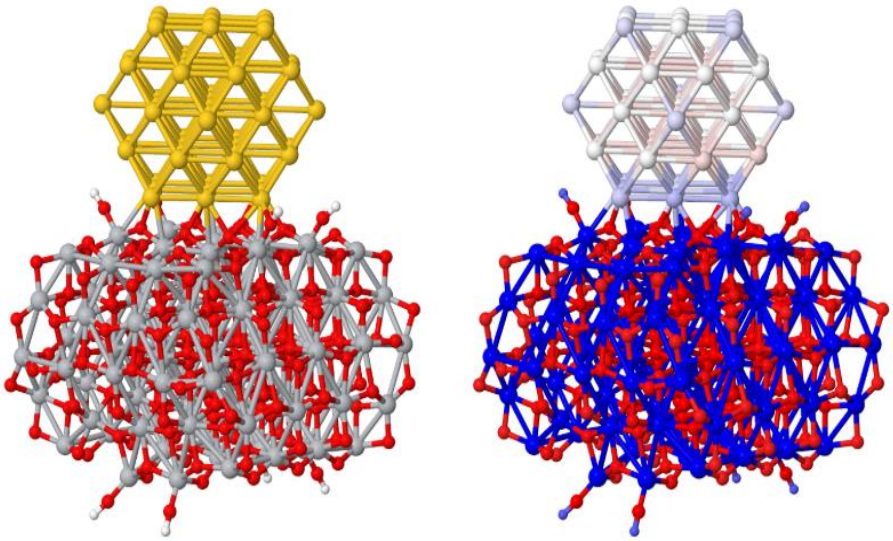
Computer modelling has become a key feature to understand and predict existing and new materials and molecules. From our extensive experience applying and developing computational models, we will illustrate through examples how computer models have evolved and yield key information on diverse problems in nanoscience such as magnetic and bottom-up nanographenes, covalent organic frameworks [1] and composites based on inorganic nanoparticles [2].



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# Graphene micro and macro electronic sensing devices

**Pedro Alpuim**[1,2*], Agnes Purwidyantri[1], Telma Domingues[1,2], Fátima Cerqueira[1,2], Sergej Tkachev[1], Pedro Marques[3], Siva Sankar[1], Marco Martins[1], Marta Prado[1], Andrea Capasso[1], Jérôme Borme[1]

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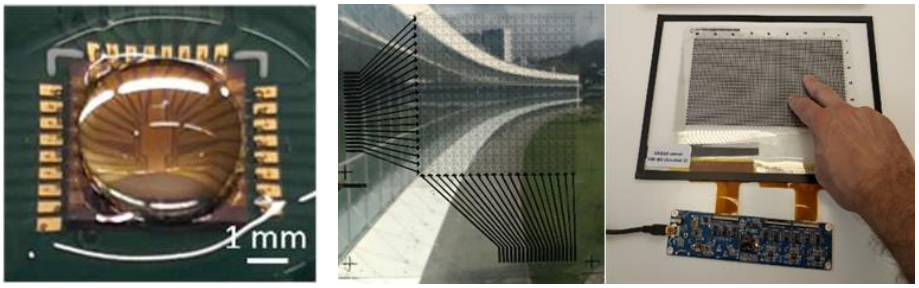
As real-life applications loom, graphene-based and other two-dimensional materials are approaching the industrial production stage [1]. Up scalable processes for 2D materials growth can be bottom-up and top-down, such as chemical vapor deposition (CVD) and liquid phase exfoliation (LFE). While CVD is particularly suitable for high-mobility single-layer graphene for micro and nanoelectronic devices, LFE methods allow for the direct deposition of multi-layered films at low cost, over large-area substrates, like those used in macroelectronics [2]. In this presentation, we report biosensing chips based on CVD graphene field-effect transistor (GFET) microelectronic arrays capable of discriminating between different Port wine grapevine varieties based on the number of SNPs that are present in the studied portion of their genome, with an attomolar limit of detection. Using LPE by high-shear mixing in the environmentally friendly, non-toxic solvent cyrene, we prepared graphene inks and extended this green approach to the exfoliation of hBN and MXenes. The graphene dispersions have concentrations above 4 mg/mL and high stability (over 9 months). Membranes were fabricated via vacuum-filtration on PVDF supports and tested in water purification technologies. The dispersions were also deposited by spray coating on flexible PET substrates to fabricate a macroelectronics 20x20 $cm^2$ multi-touch screen prototype as a proof of concept.

Figure 1 – Graphene biosensing chip (left); Graphene multi-touch screen prototype (center, right)

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# Improvement of mechanical performance of nanocomposite materials through processing: the key role of uniform dispersion of reinforcing CNTs

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This presentation intends to demonstrate the key importance of uniformly dispersing multiwalled carbon nanotubes (MWCNTs) into the matrix materials as a precondition to get the full benefits from their reinforcing potential of the pargeted matrix materials. The same principle applies to any other kind of reinforcing nanodispersoids such as graphene, graphene oxide, plate-like clayey particles of the smectite family, and anisometric or isometric nanoparticles. The benefits of colloidal processing to obtain homogenous dispersions of the different nanocomposite components were combined with those of freeze-granulation to preserve in the freeze-dried granules the high degree of homogeneity achieved in the starting suspension. This approach has been used to prepare poly(methyl methacrylate) (PMMA)-modified hydroxyapatite (HA) nanocomposite cements reinforced with MWCNTs. HA conferred bone bonding ability to this new generation biomedical bone cements, while a small addition (0.1 wt %) of MWCNTs maximized the mechanical properties of PMMA/HA nanocomposite. The same innovative colloidal approach was also successfully used to obtain a new class of closed-cell Al-foams reinforced with MWCNTs. These nanocomposite metal foams synergistically combine the remarkable properties of both metal foams and carbon nanotubes. The results indicate that the tubular structure of carbon nanotubes is preserved throughout the entire the process. The carbon nanotubes are individually dispersed, stretched and randomly aligned in the aluminum-matrix of these closed-cell foams, thus potentiating their homogeneous 3D reinforcing role. Accordingly, the overall relevant mechanical properties of the resulting nanocomposite materials were noticeably enhanced.

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# Invited speakers

# I1. Fabrication and charge transport study in Perovskite solar cell

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NiO is a well-known p-type semiconductor primarily used as Hole transport material in Perovskite solar cells. It has become a prospective candidate for HTL as its p- type characteristics of high optical transmittance (wide band gap (Eg>3.5eV)), excellent thermal and chemical stability and a relevant valence band match with common photoactive layers. The nickel acetate precursor fully decomposes and the NiO film shows larger crystalline grain sizes, which gives the better hole transport properties. Hole extraction and transport properties of NiO film interfaced with the perovskite film were higher than those of organic HTL's and perovskite deposited on NiO film is with homogeneous phase.

Nickel oxide (NiO) thin films are widely used as hole transport layer in perovskite solar cell (PSC). Hole transport materials have a great impact on efficient hole extraction in PSC, as well as the long term stability of the devices. The magnetic domains and other magnetic phenomena in surface structures of NiO thin film are studied by magnetic force microscopy (MFM). The surface morphology and topology of thin film has been studied by the atomic force microscopy (AFM) . In this paper, we report the effect of domain polarizations and the magnetic moment of NiO thin film at the interface of Perovskite solar cell. The performance of NiO in device shows the increased power conversion efficiency of 10.58%.

# I2. Exploring the strategies towards enhancing the thermoelectric performance in oxide materials

**Andrei V. Kovalevsky**[1,*], Gabriel Constantinescu[1], Diogo Lopes[1], Nuno M. Ferreira[2], Kiryl V. Zakharchuk[1], Tiago Paulino[1], Joana Zúquete[1], Diana Suarez[1], Shahed Rasekh[1], Parisa Amirkhizi[1], Andrei Galatanu[3], Myriam H. Aguirre[4], Wenjie Xie[5], Anke Weidenkaff[5]

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Oxide materials are currently considered a promising alternative to traditional thermoelectrics. Moderate charge carrier mobility stemming from strong covalent and ionic bonding, combined with relatively high thermal conductivity, represent known disadvantages of these materials for thermoelectric applications. However, oxides offer a possibility to operate at high temperatures, resulting in a higher Carnot efficiency. In addition, their known structural and microstructural versatility can open new horizons for thermoelectric applications. This work reviews some representative cases of engineering the composition and microstructure of a series of selected oxides towards high thermoelectric performance. The selected approaches will include laser processing, in situ formed composites, defects tailoring and aluminothermy-boosted sintering, also taking into account the unique redox-tuning capabilities of oxides. Representative examples will include ceramic materials based on $SrTiO_3$, ZnO, $CaMnO_3$ and $Ca_3Co_4O_9$.

# I3. Photonics Bioplastic Films for Triplet Sensitized Wideband Photon Harvesting

**Pankaj Bharmoria**[1, 2], Nobuhiro Yanai [3], Nobuo Kimizuka [3], Kasper Moth-Poulsen[1]

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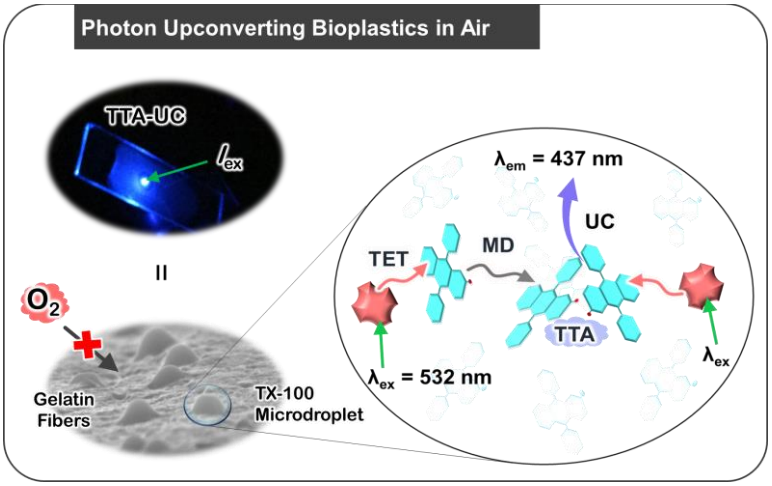
Sustainable photonics applications of solid-state triplet-triplet annihilation photon upconversion (TTA-UC) are limited by a small UC spectral window, low UC efficiency in air and non-recyclability of polymeric materials used. In a step to overcome these issues, we have developed new recyclable TTA-UC bioplastics by encapsulating TTA-UC chromophores liquid inside the semicrystalline gelatin films showing broad-spectrum upconversion (NIR/Red/Green to blue) with high UC efficiency in the air. Finally, to address the post-utility of recycling of the plastic photonics we demonstrated a proof-of-concept downstream recycling approach that gives new directions for designing future recyclable photonics bioplastic materials.



# I4. Self-assembled Peptide Nanotubes of Different Chirality: Properties and Applications

**Svitlana Kopyl** *, Pavel Zelenovskii, Andrei Kholkin

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Chirality is a property of an object to be non-superimposable on its mirror image [1]. This simple, but the universal property of matter can be observed at various hierarchical levels from subatomic, molecular, and supramolecular to macro-and megascopic scales. An interest in chirality arises first from its ubiquitous presence in living matter. A huge number of chiral molecules such as amino acids (AA), sugars, etc. exist in nature and play a crucial role in living organisms.

Self-assembly of complex molecular structures based on AA is one of the most important phenomena both in living nature and in artificial biomimetics. At the same time, the chirality of the initial molecules also plays an important role in self-assembly processes. All this is important both for our understanding of wildlife and the basic principles of the emergence of life and for numerous practical applications. Self-organized macromolecules tend to form hierarchical structures with an alternation of the sign of chirality in the transition to a higher hierarchical level. Depending on the conformation of the primary structure (L or D), the properties of the material also change. An example of such self-assembled macromolecules is peptide nanotubes (PNTs) based on various amino acids and their dipeptides. Due to their wide-ranging physical properties, PNTs are not only important in the study of biomolecular self-organization, but also show promise in various applications in the nanotechnological and biomedical fields. One example of such self-organizing macromolecules is diphenylalanine (FF) peptide nanotubes.

In this work, we will discuss the experimental and theoretical study of the structure and growth kinetics of L-FF and D-FF microtubes. A better understanding of the role of chirality in the growth process will allow for improving the methods for nanotubes and microtubes fabrication, their better implementation in various functional devices, and may assist in the development of new drugs and biomaterials [2].

Moreover, the fabrication of layered biomolecular crystals of diphenylalanine obtained via a co-assembly of L,L- and D,D- enantiomers of FF monomers is also reported [3]. Their crystal structure, thermal and chemical stabilities, and piezoelectric properties are investigated. The grown crystals demonstrate better thermal and chemical stabilities than self-assembled hexagonal FF nanotubes. Piezoelectric bilayers, being held via weak aromatic interaction in the bulk crystals, can be exfoliated by mechanical or chemical methods, thus resulting in a 2D piezoelectric material, which can find various applications in biocompatible and ecologically friendly electromechanical microdevices, such as sensors, actuators, and energy harvesting elements used in implantable and wearable electronics.

This work was 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/MEC (PIDDAC).

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# I5. Magnetoelectric coupling studies in lead-free multiferroic ceramic composites

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One of the most scientifically interesting and technologically important categories of multifunctional systems are the multiferroic (MF) materials. In its most general definition, MF compounds are those classes of materials that exhibit, in the same phase, more than one primary ferroic ordering, *viz*. ferroelectricity, ferro(antiferro/ferri)magnetism, ferroelasticity or ferrotoroidicity. Such a combination of ferroic orders, favours the possibility of coupling among them such that one ferroic property can be controlled by the other. The most striking illustration is the magnetoelectric (ME) coupling in those multiferroics that combine a non-magnetic ferroelectric (FE) with a ferromagnetic (FM) compound so that both the piezoelectric and magnetostrictive phases coexist.
This work presents a systematic study of the structural and electrical characteristics of the magnetoelectric multiferroic composites with ($Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$) [BCZT] as the non-magnetic piezoelectric phase and ($Ni_{0.7}Zn_{0.3}$)$Fe_2O_4$ [NZFO] as the non-ferroelectric magnetostrictive phase. Bulk composites with composition (1−*x*) BCZT – *x*NZFO (0 ≤ *x* ≤100 at%) were prepared using solid state reaction method. Structural and microstructural analysis using XRD, FESEM and Raman techniques confirmed the phase formation. Electrical, magnetic, and magnetoelectric (ME) measurements were performed. The composites exhibit typical well-saturated magnetic hysteresis (*M*–*H*) loops at room temperature, having very low coercive field values, indicating their soft ferromagnetic behaviour. Frequency dependence of capacitance and admittance exhibited a resonance behaviour corresponding to the radial mode of the electromechanical resonance (EMR). ME coefficients were studied in both longitudinal ($\alpha_{E33}$) and transverse ($\alpha_{E31}$) modes. The highest coupling coefficients, $\alpha_{E31}$~14.5 mV/Oe.cm and $\alpha_{E33}$ ~13 mV/Oe.cm were obtained for composite with 50 at% NZF at *off*-resonance frequency of 1 kHz. At the EMR frequency of 314 kHz, the $\alpha_{E31}$ value in 0.5BCZT-0.5NZFO composite enhanced enormously to ~5.5 V/Oe.cm.

# I6. Photoluminescence behaviour of Ho3+ with Yb3+ sensitizers in YOF nanocrystals

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Rare earth (RE) elements are prime constituents in a large amount of innovative materials and several technological advances would not be possible without their contribution. In this presentation, recent progress in the field of rare earth spectroscopy is highlighted, with a special emphasis on clean energy, sensors and telecommunications, providing a broad view on the developments.

In the many available RE based luminescent materials, rare-earth oxyfluorides (REOF) compatible for RE doping make a path for efficient near-infrared (NIR) to visible up-conversion (UC) and NIR to NIR down shifting (DS) simultaneously. The talk describes the efficient use of YOF:$Ho^{3+}$/$Yb^{3+}$ phosphor nanoparticles synthesised by the Pechini sol-gel method as multimode UC and DS in the visible and NIR (second biological window-BW-II) regions, respectively. Detailed emphasis on energy transfers, phonon assistance, decay dynamics with structural properties would be discussed with main focus on the RE luminescence and its technological importance.

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# I7. Impact of $Li^+$ ion irradiation on structural, optical, electrical and morphological properties of $BaSnO_3$ ceramics

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Barium stannate ceramics ($BaSnO_3$) was synthesized using the conventional solid-state reaction method. The precursor's barium carbonate and strontium oxide were taken in the required composition. It was subjected to calcination at 800 °C for 6 hours followed by sintering at 1400 °C for 4 hours and made into pellets. They were irradiated with Lithium ($Li^+$) ion of 50 MeV energy at a fluence of $5\times10^{11}$, $1\times10^{12}$, $5\times10^{12}$ and $1\times10^{13}$ ions/$cm^2$. The crystal structure, optical property, electrical behaviour and morphology were systematically investigated using X-ray diffraction (XRD), Fourier transforms infrared spectroscopy (FT-IR), UV- Visible spectroscopy, Photoluminescence spectroscopy, LCR meter and High-Resolution Scanning Electron Microscopy (HRSEM). The changes in the structural, optical, electrical and morphological properties of the prepared $BaSnO_3$ ceramics were studied before and after ion irradiation. The crystallinity of $BaSnO_3$ ceramics was well defined with sharp peaks revealed from powder XRD patterns that confirm the presence of cubic phase. The FTIR spectra show different modes of vibrations of molecular groups and functional groups present in the sample. UV- Visible spectroscopy has been recorded to estimate the bandgap of the prepared pellets. Photoluminescence spectroscopy confirms the luminescence behaviour of $BaSnO_3$. The dielectric spectroscopy and A. C. conduction mechanism in the prepared ceramics were studied for every 5 degrees change from room temperature to 400 °C for a frequency range of 1 kHz to 2 MHz. Dielectric constant and activation energy of the sample before and after ion irradiation was calculated. The morphology of both pristine and irradiated ceramics was analyzed using SEM images.

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# I8. Growth and ferroic physical properties of bismuth-layered magnetoelectric oxide thin films for low-loss energy-storage

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Development of environment-friendly dielectric capacitors that present the coexistence of ferroelectricity, magnetic order and the coupling between different ferroic orders with low-leakage density is a challenging task for practical electronics. Processing, chemical stability, and localized defects in ferroelectric perovskites play a key role in determining the electrical behavior at the nanoscale. Bismuth-layer structured ferroelectric oxides in this regard have the potential for magnetoelectric cross-coupling and high-temperature stability against depolarization. However, the processing of oxide thin films of higher layers (>3) is always prone to intergrowths and non-stoichiometry. The work is aimed to address such issues.

The investigation is aimed to fabricate thin films of 5-layered bismuth layered ferroelectrics to study the effect of structural strain on various ferroic functionalities. We grew Sr-containing relaxor-type oxide thin films by the pulsed laser deposition with thickness in the range of 80 - 400 nm. Growth optimization, detailed structure, chemical environment, polarization, magnetic behavior, and magnetoelectric coupling were studied. The observation of ferroic orders was analyzed with an emphasis on the structural strain and local chemical environment. The energy storage performance of the optimized thin films is presented as a function of temperature. Our thin film samples presented a magnetoelectric coefficient of 50 mV/cm-Oe and a recoverable storage density of 90 J/cm3. The experimental work demonstrated a promising environmentally benign candidate for dielectric energy storage that consumes lower energy for domain reversal at higher electric fields.

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# I9. Development of Hydrogen production reactor system utilizing Water & Zinc Indium Sulfide

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Nature plays a dual role as a survivor as well as destroyer. A quest of conquering balanced environment for the ultimate search of "Who am I" gave birth to pollution and energy crises. Photocatalytic hydrogen generation is a torch bearer in the science oriented utopian world to enhance transhumanism. In order to enhance photocatalytic hydrogen generation engineering and development of efficient and economical water splitting reaction setup is the need of the hour. In present work, an attempt is to manufacture eco-friendly, cost effective, user friendly hydrogen production setup. This setup is tested with the help of various sacrificial reagents using zinc indium Sulfide (ZIS) nanostructures along with hydrothermal synthesis reaction to produce ZIS flowers is discussed and plausible growth mechanism is proposed. The result of incorporation of benzyl alcohol (BA) as primary alcohol are striking as it serves as a scavenger in water splitting experiment reports 3013.2 µmol/h/g hydrogen under UV lamp irradiation which is almost four folds more than the ZIS catalyst without scavenger. During the photocatalytic reaction BA scavenging the photo-generated holes (. OH) and avoid the charge recombination.

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# I10. Electrochemical conversion of glycerol into energy and carbonyl compounds using microfluidic systems

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Microfluidic fuel cells (µFCs) are miniaturized systems that convert chemical energy from a fuel into electric energy by coupling a spontaneous redox reaction. The fuel is oxidized at the anode while the oxidant is reduced at the cathode, and the reactions are separated by a colaminar flow, without the need for an ionic permeable membrane. These systems exclude the ohmic resistance and the costs associated with a membrane and allow the use of mixed-media, where each half-reaction is optimized independently. These features make it possible to harvest useful energy from organics with multiple C-C bonds, such as glycerol, a massive byproduct of biodiesel fabrication. We have been developing mixed-media µFCs fed with glycerol with new anodes [1], new oxidants [2], new cathodes [3], new architectures [4], fed by exchangeable fuels [5], and producing carbonyl compounds [6]. In terms of architecture, we developed a low-cost 3D-printed µFC to replace the conventional PDMS cells [5]. In terms of oxidants, we found that HClO or $ClO^-$ can be a powerful liquid oxidant in alternative to $O_2$-saturated catholyte [2,3]. The use of HClO from bleach coupled to glycerol electrooxidation in an alkaline medium yielded the benchmark power density among all alcohol-fed µFC of 315 mW $cm^{-2}$, using Pt/C as anode and cathode [2]. In terms of materials, we found that *in situ* modification of electrodes in assembled ready-to-use µFCs builts well-dispersed and active anodes and cathodes. This strategy modifies the electrodes exactly where it is needed, increasing the collision factor of the reactants with the active sites. For instance, decorating the anode of Pt/C dispersed on carbon paper (CP) with Fe [1] and the cathode of CP with graphene oxides [3] improves overall power density. We recently showed that the use of *in situ* Bi-decorated Pt/C/CP as an anode leads to the production of glycolate and formate concomitantly to power, with a net conversion at zero bias [6]. In this context, it seems glycerol can be converted into high output power and compounds with high market prices using µFC. The future steps include scaling by *scale out* to reach the demand of high power devices and of specific markets that use small-chain carbonyl compounds in their industrial production.

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# I11. Basic principles and recent advances in photocatalytic fuel cells

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Reducing greenhouse gas emissions and implementing a renewable energy source economy are critical points our modern society needs to solve [1]. Photocatalytic fuel cells (PFCs) that concomitantly convert chemical and solar energy directly into electricity, with zero carbon emissions, have been proposed as a single device able to address both issues at once at a relatively low cost. PFC devices combine two well-defined approaches for clean energy production and fuel generation, the fuel cells (FCs) and photoelectrochemical (PEC) systems. Regardless of being new, the PFC community is growing fast, with several papers published and patents required in the literature in the last years. The present talk at ICNMSME2022 will focus on the basic principles, definitions, fundamentals, building devices, and testing half-cell reactions and performance of PFCs. Special attention will be given to recent developments and achievements in designing new and engineered semiconductor materials for efficiently harvesting solar energy and converting it into electricity and environmental remediation.

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# I12. Electronic and Magnetic Properties of Diluted Magnetic Semiconductor Thin Films: A Synchrotron based X-Ray Spectroscopic Techniques

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The study of spintronics materials such as diluted magnetic semiconductor (DMSs), multiferroic and half-metallic alloys is one of the most attractive fields in science from the viewpoints of both academic research and applications. In order to clarify the origin of ferromagnetism of these spintronics, it is necessary to investigate the electronic structure. Here, we have investigated the electronic structure of spintronics materials i.e. multiferroic materials (e.g. $BiFeO_3$) using x-ray absorption spectroscopy (XAS) and x-ray magnetic circular dichroism (XMCD).

The first discovery of room-temperature ferromagnetism in Co-doped $TiO_2$ by Matsumoto *et al.* has arisen great interest in the search for such materials and a number of studies have been carried-out to investigate whether the ferromagnetism is carrier-mediated or not, but the issue still remains controversial. XMCD at the Co $2p \rightarrow 3d$ absorption (Co $L_{2,3}$) edge is an ideal technique to clarify this issue because it is an element-specific magnetic probe. Our previous XMCD study has revealed that the ferromagnetism is not due to segregated Co metal clusters but is due to $Co^{2+}$ ions in the $TiO_2$ matrix. However, the XMCD signal intensities were an order of magnitude lower than that expected from the bulk magnetization. We performed XAS and XMCD studies on rutile Co-doped $TiO_2$ by the surface-sensitive total electron yield (TEY) mode and the bulk-sensitive total fluorescence yield (TFY) mode and found that Co ions in the bulk indeed have a large moment of 0.8-2.2 $\mu_B$ /Co. Then we extended the same approach to anatase Co-doped $TiO_2$ and studied the correlation between magnetism and transport properties.

# I13. The comparative study of mechanical properties of armchair and zigzag borophene nanotubes

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Recently, the study of nanotubes has been interested due to their new and strange behaviour. In this investigation, the mechanical properties of armchair and zigzag borophene nanotubes [1] were studied. The molecular dynamics simulation technique at the NPT (constant number of atoms, pressure and temperature) ensemble used to study armchair and zigzag borophene nanotubes based on reactive force-field (ReaxFF) interatomic potential [2]. We used the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [3] to investigate the effect of stress rate, nanotube diameter, and temperature on the mechanical properties of borophene nanotube, including the Young's modulus, Poisson's ratio, toughness and stress-strain diagram. The results showed that borophene nanotubes have different mechanical properties in the direction of armchair and zigzag, which indicates the anisotropy of borophene nanotube.

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# I14. Firing and post-firing processes of historic Mg-rich calcareous bricks

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A representative type of brick that shapes the built heritage of the city of Padua (Northern Italy) has been studied by means of a multi-analytical approach, consisting in spectrophotometry, X-ray fluorescence (XRF), powder X-ray diffraction (PXRD), polarized light optical microscopy (POM) and high-resolution scanning electron microscopy (HRSEM-EDS). Mg-rich calcareous illitic clays were used and high temperatures -from 900 to over 950 °C- were reached. The main firing processes were the profuse nucleation of pyroxene-type crystals within a widely extended Ca-aluminosilicate amorphous phase and the transformation of the original Mg-rich clayey grains to Mg-silicate mineral phases. A high reactive and supersaturated meta-stable system and a firing technique where the rapid heating and/or soaking of bricks took play are suggested. Zeolite and calcite secondary phases crystallized after firing. The former was enhanced by the high calcium content of the ceramic bodies and the high humid conditions of the city, and the later was chiefly formed from calcareous solutions. Both firing and post-firing processes have boosted the conservation of the bricks. Hence, the Ca-rich amorphous phase and the pyroxene-type phases have provided strength to the bodies and the porosity yielded by the firing of the carbonate-rich clays was largely filled by secondary calcite, increasing the cementation of the bricks. The results achieved may be transfer to current ceramic industry to produce highly resistance bricks from Mg-rich calcareous clays and especially suitable for humid environs.

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# I15. New piezoelectric in Pirydyl-Alanine based hybrid crystal

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New amino acid based [3-(4-pyridyl)-Ala-OH][$BF_4$] (hereafter abbreviated as 4PyAla), crystal was synthesized and its structure and functional piezoelectric properties were investigated in detail. 4PyAla crystallizes in the polar $P2_1$ space group. Piezoelectric force microscopy (PFM) measurements revealed that polarization of the sample of 4PyAla is vertically oriented. The crystal structures of crystals under investigation are characterized by inter- and intramolecular hydrogen bond networks. The existence of intramolecular hydrogen bonding was confirmed by means of IR measurements. The thermogravimetric (TGA) technique was applied to study the thermal behaviour of the title crystals. The piezoelectric properties are discussed in the context of the crystallographic structure and the microstructure of the crystals.

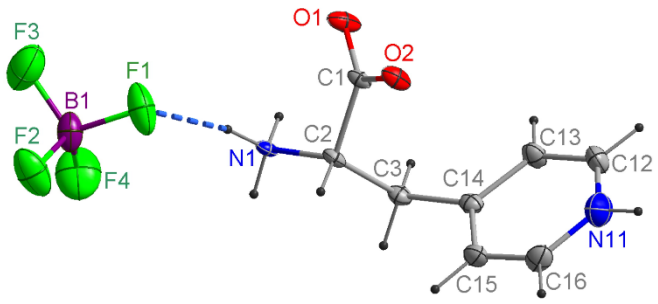


Fig. 1 The molecular structure of compound (abbr), showing the atom-numbering scheme and N–H•••F interaction (light blue dashed line). Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

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# I16. Use of CVD Diamond films to improve the thermal management of GaN high electron mobility transistors: an historical overview

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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. In order to guarantee that the operating temperatures are kept within reasonable limits, the heat generated at the active regions of a device needs to be transferred to the package, where it can be ultimately dissipated to the heat sink or external environment. This requires 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 thermal conductivity, bandgap and breakdown electric field, diamond can be considered the ultimate thermal management material. Diamond plates are commercially available to the engineer and this material can also be grown on a variety of substrates by chemical vapor deposition. This flexibility allows for different possibilities of integrating it within a package. The use of artificial diamond films for the thermal management of power devices, such as p-n junction diodes, LEDs and transistors, has been an active research topic for several decades. The integration of GaN high electron mobility transistors (HEMTs) and diamond films, in particular, is one of the most successful approaches and has involved academic and industrial institutions for more than 20 years. The integration of both materials can be done in two ways: replacing the GaN substrate with diamond or capping the HEMT with a diamond film, close to the gate hotspot. The GaN-on-diamond wafers can be obtained by depositing the diamond film directly on the back of GaN layers, following the substrate removal, by bonding GaN HEMT wafers and diamond substrates, and by growing the GaN layers directly on diamond substrates (GaN epitaxy). This paper will describe each of these approaches, their challenges and their benefits, and will present the evolution of the GaN/diamond devices reported by different groups.

# I17. High temperature wet chemical synthesis of two dimensional chalcogenide nanosheets for photodetector applications

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This work analyzed the effect of Different high boiling point solvent combinations in the synthesis and photo-sensing characteristics of Tin Disulfide (SnS2) thin nanosheets. Well-characterized samples were employed to fabricate heterojunction photosensitive diode, and their performance was presented in detail. Solvent dependency in the synthesis and single-phase formation were observed using powder x-ray diffractometry (XRD) and was verified with Raman spectroscopy measurements. Particles synthesized with only Oleylamine show mixed-phase, and two other solvent combinations such as Oleylamine+Oleicacid+n-Octadecene, and Oleylamine + Oleic Acid shows single-phase 2H-SnS2 without phase contamination. Transmission electron microscopy was used to verify that the formed sheets are nanosheets with lotus leaves and hexagonal shape-like morphology. Well-characterized samples were employed to fabricate a heterojunction photosensitive diode using a p-type silicon substrate. Light-responsive measurement results of fabricated diodes indicate that Oleylamine + Oleic acid synthesized sample shows very high light sensitivity; the fill factor value of the fabricated diode is closer to the ideal diode.

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# I18. Role of the molecule's conformation on the piezoelectric properties of diphenylalanine nanostructures

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Piezoelectric properties of organic materials are closely related to molecular dipole moments and their spatial packing. The role of vectored forces on the packing of small aromatic peptides and the correlation between their structure and properties were studied recently [1,2]. Molecular packing, in turn, is closely related to the conformation of the molecules, which also determines polar properties of the molecules. Though most of biomolecules possess nonzero dipole moment, in a crystal, this moment can be reduced due to an improper molecular conformation. Here, by means of quantum chemical calculations we studied the effect of the molecular conformation on the polar properties of diphenylalanine (FF) dipeptides and their evolution in different nanostructures. We demonstrated that the highest dipole moment of FF is observed for *trans*-configuration, whereas the most stable conformation is *cis*. The main source of the dipole moment of FF is zwitterionic charges, whereas aromatic interaction between phenyl rings serves for stabilization of the configuration. At the same time, less stable *trans*-configuration is more flexible and can form higher diversity of crystal structures, though little of them demonstrate noticeable piezoelectric properties. The obtained results uncover the role of molecular conformation on the functional properties of molecular crystals and also provide an additional functionality for the design of organic piezoelectrics. This work was 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/MEC (PIDDAC). P.Z. and A.K. were supported by FCT Project PTDC/CTM-CTM/4044/2020.

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# I19. Reduced graphene oxide biomaterials as a potential therapy for spinal cord injury repair

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In general, patients suffering from severe organ failure can be treated with transplanted organs[1]. However, in the case of the central nervous system this is not yet possible, as happens with patients of spinal cord injury (SCI). Research-based approaches are currently focused on the use of cells, drugs and biomaterials[2]. For instance, a popular strategy for spinal tissue healing consists of the design of 3D biomaterials to fill and stabilize the lesion cavity, acting as a support and guide of the different neural tissue components. In this work, two kinds of 3D scaffolds made of reduced graphene oxide (rGO), in the shape of foams and microfibers, were chronically implanted in the right hemisected cervical spinal cord (C6 level) of a rat experimental model of SCI[3,4]. *In vivo* biocompatibility, in terms of behavior affectation along with systemic and local tissue responses, was thoroughly studied four months after their implantation following an interdisciplinary approach. Results indicated that both kinds of scaffolds, without any further biofunctionalization, facilitated the creation of a more regenerative scenario. Implants fostered the stabilization of the injured spinal tissue, as well as the presence of neuronal structures along with blood vessels at the lesion epicenter. Moreover, rGO foams reduced perilesional damage as well as caused harm in the contralateral hemicord and rostral/caudal regions. Indeed, their presence modulated the inflammatory response. Finally, rGO materials did not affect rat spontaneous behaviour or induced systemic toxicity in major organs. Taken together, these results demonstrate the promising potential of rGO scaffolds as neural interfaces capable of fostering the repair of the injured spinal cord. Current efforts are also being made to understand which neural cell populations could be implied in spinal tissue restoration for further material functionalization.

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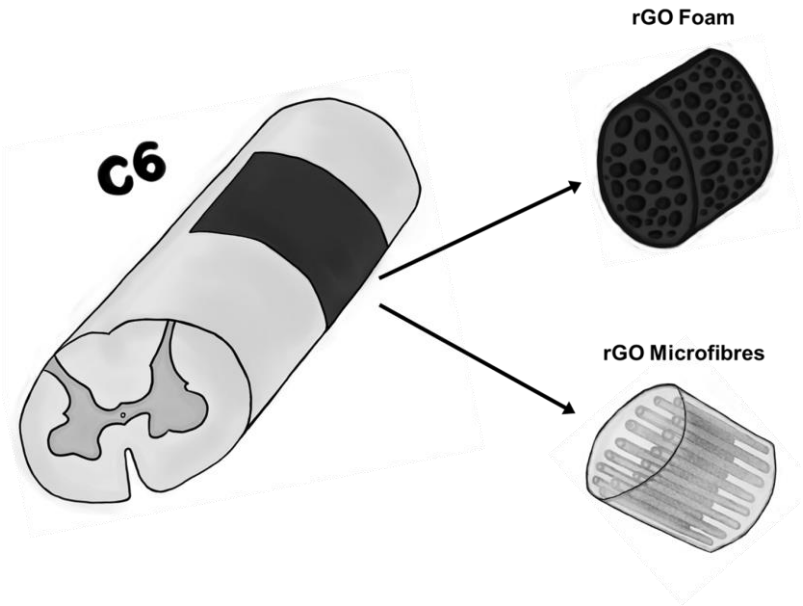


**Figure 1: rGO implants.**

# I20. Diverse Optical thermal sensing mechanisms in rare earth activated Aurivilliu's family compound

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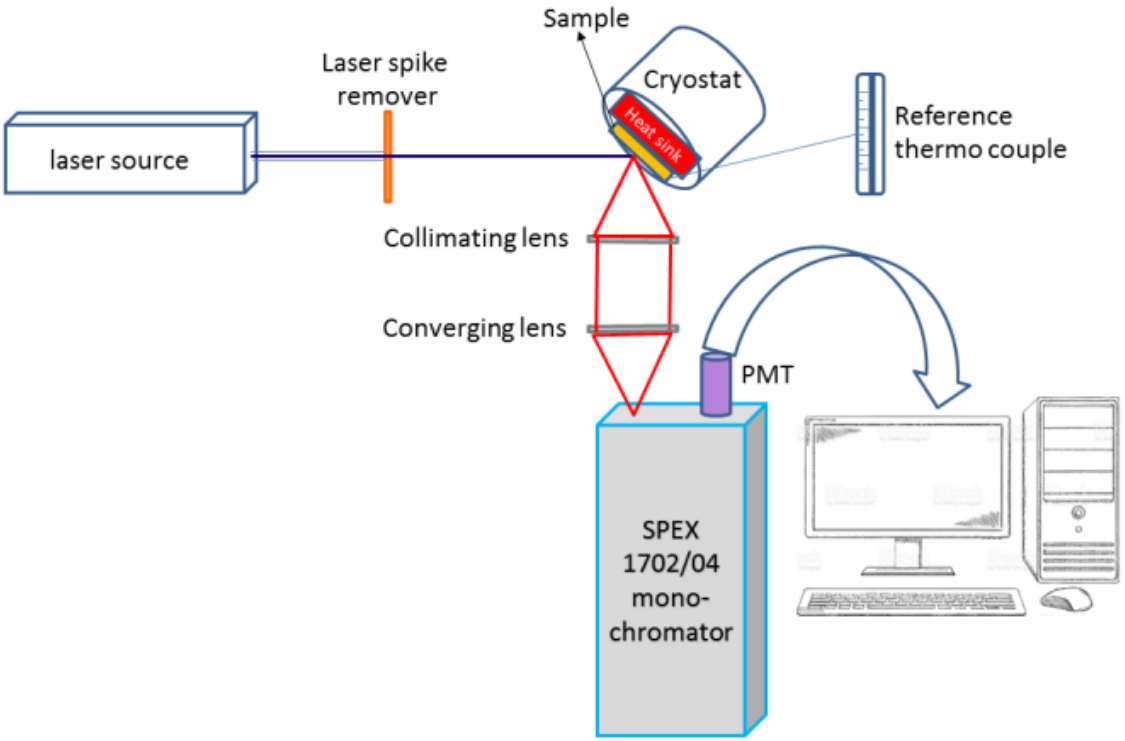
Luminescence based temperature sensing is one such kind of applications with modern light based application apart from direct display applications such as phosphors, scintillators, photocatalysis and others. Luminescence based thermometry has an enormous potential not only in in vitro and in vivo bio-imaging and medical treatment but also in the fields of temperature distribution and maintenance in vast surface areas such as electronics, aviation, space research etc.,




Several methods of optical temperature sensing were established in the recent years and vast research has been done on each of them. It has been proved that a single material could be used for thermal sensing through various methods. The requirements of optimized luminescent thermometers are their thermal sensitivity in the range of temperatures to be examined besides their accuracy, repeatability, and stability of the material in the ambiance of measurement. Depending on the measurement conditions the range of operating temperatures are defined. Hence, few phosphors with good sensitivities are not enough for the entire ranges and applications. Wide range of phosphors with varied physical, chemical, and even mechanical properties with excellent sensitivities in defined range of temperatures are very much needed. The presentation

describes different approaches in sensing temperature via non-contact approach using diverse optical thermal sensing behaviour of $Er^{3+}/Yb^{3+}/Tm^{3+}$ co/tri-doped thermally stable compounds of Aurivilliu's family, bismuth lanthanum tungstate (BLW) phosphor. The dependence of the integral intensity of luminescent ions as a function of temperature was monitored in cryogenic temperature range. Three methods of thermal sensing, namely fluorescence intensity ratio (FIR) based on thermally coupled levels (TCL) and thermally non-coupled levels (NTCL) in the visible upconversion were discussed by comparing the sensitivities of each of the method based on theoretical interpretation of the results. Various temperature sensing techniques were implemented, and corresponding absolute ($S_A$) and relative sensitivities ($S_R$) were estimated to compare.

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# I21. Consequence of graphene oxide to reduced graphene oxide transformation on the hydrogen storage behavior of GO/$MgH_2$ composite

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Development of a hydrogen fuel tank, which can deliver >5.5 wt.% $H_2$ for 1500 cycles at temperatures <85 °C and pressures 5 - 12 bars, is crucial for making the hydrogen vehicle program a practical reality [1]. High-capacity light weight metal hydrides receive attention for this purpose, but it is not yet possible to identify a reversible hydride with the required features for storing hydrogen. The only close contender is magnesium hydride ($MgH_2$), but the main issue is that >350 $^oC$ is required for the liberation of hydrogen [2]. Recently, the current team has demonstrated that the hydrogen desorption temperature of $MgH_2$ can be lowered substantially by incorporating suitable additives, especially metal oxides. In this context, our interest for the current investigation is graphene oxide as additive for $MgH_2$. We observed that when a small amount of GO (5 wt.%) is ball milled with $MgH_2$, mild reduction occurs during mechanical milling itself, whereas a strong reduction of GO happens concurrently with the formation of MgO. Due to the transformation of GO to rGO, the powder releases hydrogen by at least 60 $^0C$ lesser temperature and the kinetics improves by two orders of magnitude. The GO to rGO transformation leads to the lowering of dehydrogenation activation energy ($E_a$) barrier >20 kJ/mol and its apparent consequence is, improved dehydrogenation of $MgH_2$ at low temperatures. We have also analyzed the GO-$MgH_2$ composite samples extensively by differential scanning calorimetry (DSC), X-ray diffraction (XRD), Raman spectroscopy, Fourier transform infrared (FTIR) spectroscopy and atomic force microscopy (AFM) techniques. All these tests suggest that GO to rGO transformation is the key factor for the improved catalytic activity of heat-treated GO/$MgH_2$ composite powder.

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# Oral presentations

# O1. Green synthesis of metal sulphide nanoparticles: Morphological, chemical, optical properties and activity as nanofertilizers

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Metals sulphides have interesting chemical and physical properties, Due to that, Metal sulfide nanomaterials have attracted great attention [1]. They have been studied and investigated for use in batteries, catalysts, light emitting diodes, solar cells, and many other fields currently they are also being studied in Agriculture as nanofertilizers. This is mainly due to the fact that sulphur is one of the essential nutrients for plants and metal sulphides are known for their anti-microbial and anti-bacterial and antifungal activities [2]. Metal sulfide nanostructures have been synthesized by a variety of chemical or physical methods. Currently, there has been an increased emphasis on the topic of "green" chemistry. In this study metal sulphide nanoparticles were synthesized through the green route. Plant extracts were used as reducing agents [3]. Metal nitrate salts, metal sulphate and Thiourea were used as metal and Sulphur source respectively. The optical properties of the synthesized nanoparticles were studied using UV-Vis and characterized using SEM, TEM, XRD, and FTIR. And the nanoparticles were then studied as nanofertilizers.

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# O2. New approach to the molecular electronics of fluorographene

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Among the graphite oxide models [1], two predict planar structures (Hofman and Lerf-Klinowski). In this research a graphene model is proposed that allows an interpretation of different characteristics of fluorographene such as: the maintenance of the quasi-planar structure, stability of non-stoichiometric fluorographene [2], dispersibility of fluorographene in solvents with a large closed conjugated system formed by $p_z$ orbitals[3], presence of the semi-ionic bonds between C and F revealed by the characteristic peaks in C1s XPS [3], diversification of the C-F bonds between the two sides of the layer which produces apparent destruction of the planar structure between the carbon atoms.

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# O3. Lithium titanium phosphate materials for Li-ion batteries: study of the grain boundary properties with boron addition

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In this work, we study the effects of 20 mol% boron addition to the lithium titanium phosphate solid electrolyte composition ($Li_{1+x}Ti_{2-x}B_x(PO_4)_3$) for application in Li-ion batteries. We compare the structural, microstructural, and electrochemical features of the unmodified ceramic ($x$ = 0, designated as LTP) with the boron-doped composition ($x$ = 0.2, designated as LTBP20). Ceramic compacts of both LTP and LTBP20 samples were made by firing uniaxially pressed samples at 650 °C and 850 °C, respectively. Electrochemical impedance spectroscopy (EIS) revealed that both bulk and grain boundary conductivities are significantly enhanced in the LTBP20 sample, in agreement with the higher $Li^+$-ion concentration determined from the analysis of the XRD patterns. The space charge properties of the grain boundary region were then determined, revealing that the level of the depletion of $Li^+$ charge carriers is less severe in the LTBP20 sample. Overall, this work provides new insights on the electrochemical characteristics of the grain boundary of NASICON-based solid-state electrolytes, which has been often overlooked in the literature [1,2].

**Acknowledgements**

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# O4. New Plasmonic-Magnetic Nanomaterials for Shell-Isolated Nanoparticle-Enhanced Raman Spectroscopy (SHINERS)

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The analysis of surface of various materials is important both from the economic and scientific points of view. Such analysis is especially difficult for so-called buried interfaces, which include interfaces of various biological samples in their “natural” environment. Many techniques standardly applied for surface analysis (especially those utilizing beams of electrons) require a high vacuum above the surface being analyzed. Unfortunately, when introduced into a vacuum, many types of biological samples suffer significant damage (it means that *in situ* characterization of surfaces of various biological objects is usually not possible using many standard surface science techniques). In 2010, Li *et al.* showed that various surfaces (including surfaces of some biological objects in the in situ conditions) may be easily analyzed using a modification of surface-enhanced Raman scattering (SERS) spectroscopy, so-called shell-isolated nanoparticle-enhanced Raman spectroscopy (SHINERS) [1]. In SHINERS measurements, the surface which is analyzed is covered with a layer of plasmonic nanoparticles (formed from gold, silver or alloys thereof) protected by a nanometric-thick layer (usually formed from a relatively inert oxide such as $SiO_2$, $Al_2O_3$, $MnO_2$, $ZrO_2$, or $TiO_2$), and then the Raman spectrum of the investigated sample is recorded. In this contribution the first examples of synthesis and applications of magnetic SHINERS nanoresonators will be presented (e.g. Au@$Fe_3O_4$ [2] or $Fe_3O_4$@Au@$SiO_2$). Such materials can be very easily deposited homogeneously on the analyzed surfaces using the following simple procedure: deposition of a drop of a sol of magnetic SHINERS nanoparticles and evaporation of the solvent when the sample is placed in a magnetic field. Examples of analyses with the use of such SHINERS nanoresonators will also be presented.

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# O5. Photocatalytic degradation of toxic pollutants from waste-water by thermally-modified Graphitic Carbon Nitride

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Water pollution is one of the greatest concerns of the present world which needs immediate attention and strict regulatory measures to prevent its paramount adverse effects on the environment. Chemical pollutants like colored dyes and heavy metals are discharged from countless industries like textiles, tanneries, and pharmaceuticals which contribute extensively to contaminating freshwater resources of this planet whereby causing deleterious effects on all living organisms including human beings. Graphitic carbon nitride (GCN), comprised of carbon and nitrogen, is a distinctive material that procured massive prominence in recent times owing to its prospective applications in numerous practical fields, including wastewater purification. Substantial porosity and surface area, non-toxic nature, low-cost and high-yield of production along with notable stability and durability are some of the remarkable features possessed by GCN which in turn make it a promising contestant for catalytic activities. The present work reports the synthesis of thermally modified GCN by two-step thermal treatment procedure and its subsequent utilization in the photocatalytic reduction of toxic pollutants like Rhodamine B dye (RhB) and chromium ions ($Cr^{6+}$) from water environment. The as-synthesized exfoliated GCN (GCNX) was characterized by different techniques like XRD, FTIR, XPS, BET, DRS, PL and TEM to elucidate the phase formation, chemical structure, surface area, optical properties and morphology of the sample. GCNX was able to degrade RhB dye within 30 min of visible light irradiation in presence of $H_2O_2$ whereas the same sample could effectively reduce $Cr^{6+}$ to $Cr^{3+}$ within less than 2 hr. in presence of Formic acid (FA) and visible light source. Variations in different catalytic parameters were performed to study their effects on the degradation activity of GCNX. These include variation in catalyst amount, pH, initial RhB or $Cr^{6+}$ concentration, variation in $H_2O_2$ or FA concentration etc. Moreover, the effect of various salts present in water was also analyzed. The GCNX catalyst was reused for several catalytic cycles to study the stability of the catalyst. Thus the modified GCN could be effectively employed as a low-cost material for waste-water remediation.

# O6. Experimental Evaluation of Metal foam for design as a bearing Damper Replaced Old Squeeze Film Damper

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The study of metal foams and their applications towards different disciplines have increased in the last few years. Metal foams materials energy absorption, thermal insulation and damping resistance will make it a special item for new development in rotor vibration control. The vibration of a shaft supported by ball bearings are analyzed based on metallic foams. Modern gas turbine engines typically utilize squeeze film dampers (SFD) as a flexible damped support to attenuate vibration amplitude and to reduce transmitted forces. The mechanical and damping properties of metal foams will be used as a damper absorber to reduce the vibration of a simple Jeffcott rotor system. This paper aim is to explore the characterization of metal foam as a source of dampening in simple Jeffcott rotor system. also, to reduce the detrimental vibration effect on rotor dynamics supported specially by ball bearing with squeeze film metal foam damper. Among the best choices to achieve this overall objective is to propose a simple Jeffcott rotor to vibrational study behaviour means vibration analysis. The adapter covering the outer rings of the ball bearings will be modified to obtain a vibratory analysis with or without the use of porous metal foam damper as modified for old squeeze film damped. The vibration transmissibility through the metallic foam sample will be presented to figure out the damping coefficient and vibration insolation efficiency and resonance suppression during dynamic testing.

# O7. Corrosion Inhibition using ethanolic extract of a Ficus elastica in 1M HCL

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This work is part of the valorization of the ethanolic extract of the Ficus elastica leaves of the Skikda region as an antioxidant and corrosion inhibitor of X42 Grade B steel because of his various applications in the oil industry. Phytochemical screening of this extract revealed the presence of Polyphenols, Tannins, Flavonoids, Reducing Compounds, Terpenoids, Anthracenosides. The methods used to measure the antioxidant activity in this research are free radical scavenging using the DPPH and the ferric ion reducing power (FRAP), whereas for the anti-corrosion action gravimetric techniques, evolution of free potential and electrochemical impedance spectroscopy were used to study the behavior of the metal in the absence and presence of the extract. The results obtained showed that this extract exhibits an important antioxidant activity. For the latter, the inhibition obtained by electrochemical impedance spectroscopy is 81.41% with 1M HCl

# O8. A novel conductive PEDOT:PSS/GG hydrogel electrolyte based dye sensitized solar cell

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The use of liquid electrolytes in dye-sensitized solar cells (DSSCs) has some disadvantages such as evaporation and leakage of the electrolyte. The quasi-solid-state approach has been developed in recent years to overcome these disadvantages, especially for DSSCs that need to remain stable outdoors for long periods [1–3]. This study aimed to investigate the use of PEDOT:PSS/GG hydrogel as an innovative quasi-solid electrolyte in the DSSCs. Photoanode was prepared by coating the pre-synthesized $TiO_2$ on FTO using the doctor blade method. PEDOT:PSS (wt. 5%) was added to the GG polymeric solution; it was mixed in sealed containers and homogenized, and then taken into molds while hot. PEDOT:PSS/GG hydrogels, which were brought into the desired molds while hot, were left to dry at room temperature. Hydrogel-electrolytes were obtained by immersing the dried hydrogels that were cut in accordance with the cell size into the pre-prepared $I^-/I_3^-$ electrolyte solution. The measurements were carried out by forming a sandwich type solar cells with the prepared PEDOT:PSS/GG hydrogels $TiO_2$ photoanode and Pt coated counter electrode. Impedance analysis and current-voltage (I-V) characteristics of DSSCs were performed under 1000 W/m$^2$ light intensity. Power conversion efficiencies of standard liquid electrolyte and hydrogel electrolyte cells were obtained and compared. In addition, the stability of the obtained PEDOT:PSS/GG hydrogel electrolyte-based dye sensitized solar cells up to 168 h was investigated. The prepared PEDOT:PSS/GG electrolytic hydrogel is also promising for use in the field of flexible dye-sensitized solar cells.

**Acknowledgments:** This work was supported by the Scientific Research Projects Commission of Sakarya University (Project number: 2021-9-33-89).

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# O9. Passive methods in heat transfer enhancement over heated blocks using airfoil generator

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In recent decades, the industrial technologies become more powerful and more compact; heat transfer enhancement techniques are needed to evacuate the energy delivered. The passive methods can be useful to designers to enhance heat transfer in such applications. Passive heat transfer augmentation methods do not use any external power input or maintenance. One of the ways to enhance heat transfer performance in passive method is to increase the effective surface area and residence time of the heat transfer fluid [1].

Many works used the insertion of protuberant bodies to increase heat transfer in industrial systems however, they always accompanied by a drastic increase in pumping power [2, 3].

The purpose of this work is to examine the efficiency of installing airfoil-shaped disturbances to improve heat transfer without dangerously increasing the pressure drop (Fig 1).

The unsteady governing equations are solved by the finite volume method using the CFD Ansys Fluent® commercial code.

In terms of efficiency, the placement of the airfoils leads to a significant improvement in heat transfer, about twice as much as the case without airfoils. Although the installation of airfoils above the blocks increases the pressure drop, the gain obtained in the heat transfer enhancement is very high, which makes it a very interesting technological solution compared the classic used inserts.

The presence of the airfoils causes an early bifurcation of the flow to the unsteady regime at relatively low *Reynolds* number values (Re <1000). The *Strouhal* number of the obtained oscillatory flow decreases with increasing *Reynolds* number. Propagating waves further improve the fluid mixing and thus attenuate its temperature, leading to a more significant increase in heat transfer.

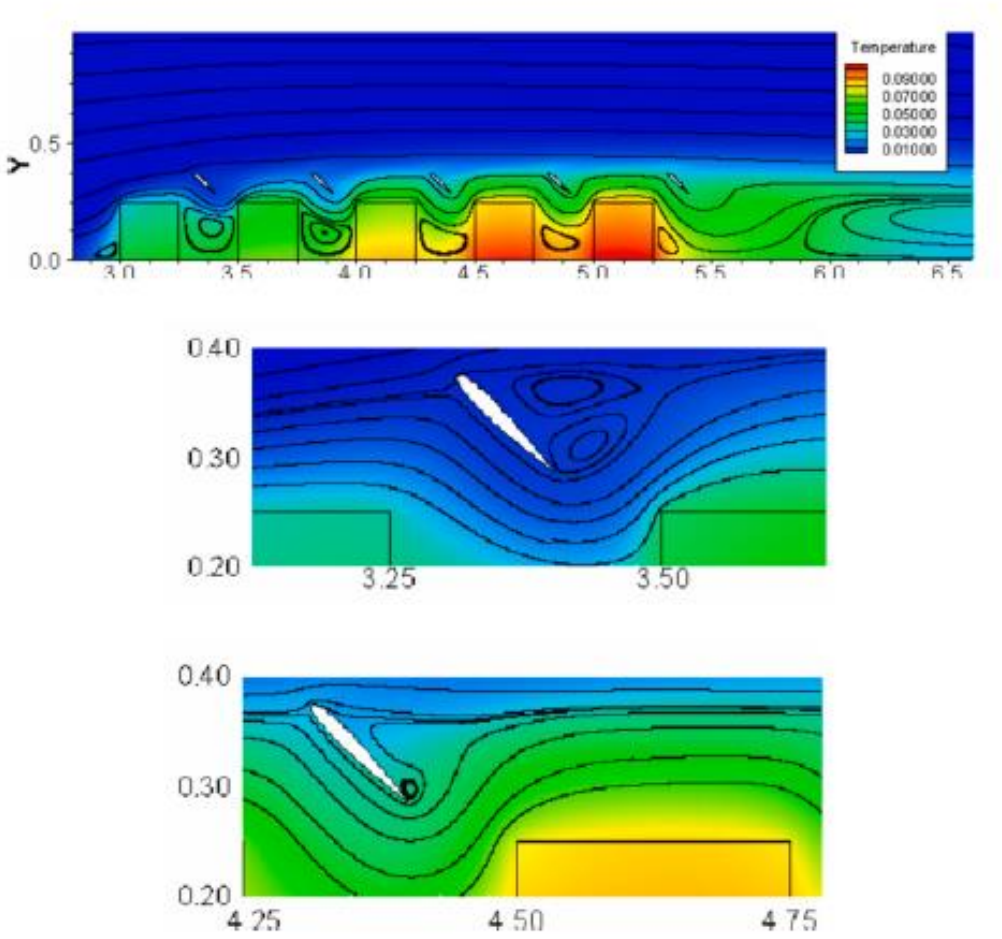


**Fig 1 Streamlines and isotherms field for Re = 500.**

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# O10. Performance Analysis for the Improvement of Worn Hydrodynamic Journal Bearings with Nano-Fluids used in Heavy Industrial Machinery: A Numerical Simulation Approach

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Nanolubricants are oils containing nanoparticles as additives to enhance the performance of journal bearings. Hydrodynamic journal bearings can be described by the Reynolds Equation accompanied by a formula for the fluid film thickness. In this case, we are working on a hydrodynamic journal bearing with a worn-out surface interacting with nanoparticle additives included in the lubricant. The equations were discretized and solved in MATLAB by an iterative method. The static and dynamic performance characteristics were calculated by running the MATLAB code on different worn depths, eccentricity ratios and viscosities of the lubricant with nanoparticle additives which are corresponding to various weight conc. and temperatures. The performance characteristics and fluid pressure distributions were evaluated for two different nano-additives, CuO and $Al_2O_3$, with varying temperatures and nanoparticle concentrations. By performing simulations with different combinations of input parameters, we find out that the nanoparticles enhance the life cycle and efficiency of worn hydrodynamic journal bearing. In our study, we also find out that CuO as a nanoparticle additive in the lubricant is more efficient than $Al_2O_3$, although both the additives perform well and give satisfactory results.

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# O11. Effect of the orientation of urban streets canyon compared to the principal axis of wind on the dispersion of pollutants in the cities

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The problem of air pollution in cities has become a concern for the future and the development of large urban cities. In order to study the physical processes involved in their transport, diffusion and accumulation [1], CFD tools have been developed. These tools are capable to simulate the flow structure and pollutants dispersion in complex urban configurations [2]. In this work, the flow characteristics and pollutant dispersion around building are investigated numerically using three RANS turbulence closure models, i.e. Standard k-ε model, Realizable k-ε and RNG k-ε model. Two 2D physical configurations are considered in a first study: a single isolated obstacle and two obstacles forming an idealized canyon street. A 3D configuration consisting of four obstacles placed perpendicular to the main axis of the wind [3] and oriented at incidence of 45° to the main axis to determine the effect of street orientation on concentration rates.

Numerical simulations are performed with OpenFOAM®source code which uses the finite volume method to solve the transport equations of mass, momentum, turbulent kinetic energy and turbulent dissipation rate. When numerical results were compared to wind tunnel experiments, it was found that the RNG k-ε turbulence model yielded the best agreement with experimental data. Moreover, the coefficients of the RNG k-ε turbulence model were adapted to better predict the flow characteristics in the urban boundary layer. The results obtained using the appropriate model show good agreement with experimental measurements for velocity flow profile and turbulent kinetic intensity. The prediction of pollutant dispersion reveals that in addition to the Reynolds number, the emission location plays an important role in the pollutant concentration distribution.

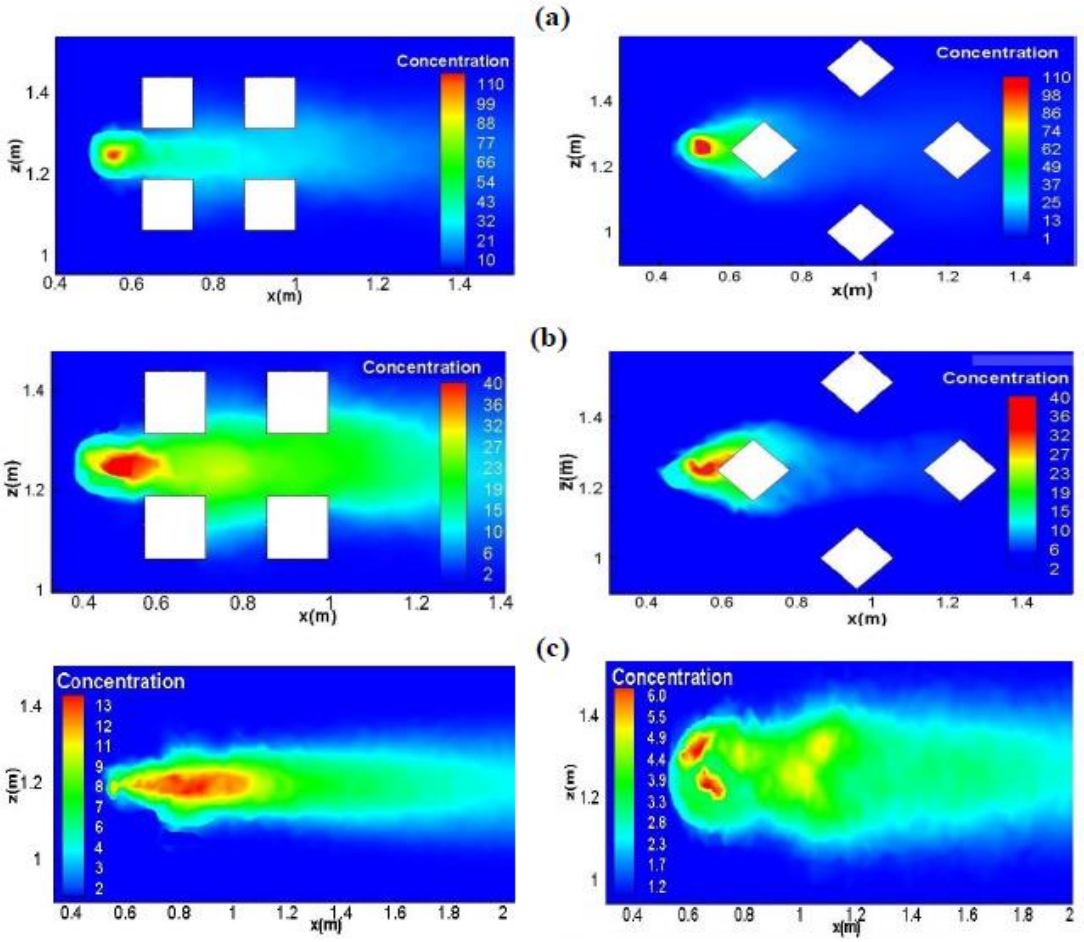


**Fig 1. Comparison of pollutant concentration values for a source located upstream of the obstacles for the case of 4 blocks aligned and oriented a) at ground level b) in the middle of obstacles c ) at level roofs.**

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# O12. The growth of Cu thin film on stepped Si (001) substrates: Molecular dynamics study

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To understand the factors that influence the growth of thin film on metal substrates with steps, and to overcome the difficulty of understanding structure at the atomic scale, some research have been developed in the epitaxial growth of Cu (001) layers on Si (001) surface **[1],** the morphology and surface property **[2]**, the temperature effect **[3].** The deposition on complex substrates is not well investigated, only some few researcher that are interested in the deposition on substrates containing a trench **[4]**.

In this work, we present the deposition of Cu on Si (001) stepped substrate. More precisely, we have studied the deposition on three different stepped surfaces. This specific investigation is performed using the molecular dynamics simulation combined with the modified embedded atom method to describe the interaction between different atoms. Our results show that the step thickness has an important effect on the morphology of the obtained film, which is quantitatively studied by the surface roughness. On the other hand, the interpenetration of the Cu atom in the different parts of the Si-stepped substrate is not the same.

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# O13. Electrodeposition of manganese sulphide (MnS) thin films : characterization and chelating agents effect

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Manganese sulfide (MnS) is a promising candidate material for an optical window or buffer material in solar cells. Thin films of manganese sulfide were electrodeposited at room on fluorine doped tin oxide (FTO) substrates. Manganese sulfate($MnSO_4$) and sodium thiosulphate ($Na_2S_2O_3$) were used in aqueous solution as precursors, with the addition of different complexing agents to slow the deposition rate of Mn. The crystalline structure, chemical composition, morphologic and optical properties of the electrodeposited thin films have been investigated.

X-ray diffraction results have indicated that all electodeposited films have cubic α-MnS structure and a crystallite size, ranging between 287.41 and 595.35 Å, depend strongly on the nature of the additive complexant. Quantitative analysis by energy dispersive X-ray technic showed that the addition of complexing agents, such as ethylene diamine tetra-acetic acid ($C_{10}H_{16}N_2O_8$, EDTA) and triethanolamine ($C_6H_{15}NO_3$, TEA), had improved the stoichiometry. SEM images indicated that the films morphology was highly influenced by the complexing agent, the addition of TEA and EDTA leads to the decrease of the grain size. Optical characterization revealed that the band gap of the prepared films, was ranging from 3.94 to 4.06 eV. It can concluded that the complexing agent TEA provides the best properties of MnS films which make it as a suitable window layer in solar calls.

# O14. Flame retardant and hydrophobic PVDF/[Imim][PF6] membranes elaborated by electrospinning method

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Electrospun membranes are highly porous materials with superior properties and are used in many advanced applications. However, electrospinning involves the application of solvents that are in some cases toxic, so it is necessary to look for more ecological alternatives such as ionic liquids. The objective of this investigation is the elaboration of a novel flammable and hydrophobic electrospun membranes based on (polyvinylidene fluoride) PVDF and the ionic liquid [Imim][PF6]. Different amounts of the ionic liquid (1, 3 and 6 wt%) were used to study the possible changes that may occur during its addition to PVDF. The electrospun PVDF/[Imim][PF6] membranes morphology and structure were examined by SEM (Scanning Electron Microscopy), EDX (Energy Dispersive X-ray Spectrometer) and FT-IR spectra (Fourier transform infrared). Mechanical properties, flammability, thermal stability, and water repellency of the developed membranes have also been investigated. Results showed that the PVDF/[Imim][PF6] electrospun membranes with 3% of [Imim][PF6] has good mechanical and flammability properties, and it is hydrophobic with a contact angle of 100.4°.

# O15. Zinc migration and its effect on the functionality of electrospun PVDF antibacterial nanofilms incorporated with ZnO nanoparticles

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Metal oxide nanoparticles represent a promising potential for the development of new antibacterial materials, including zinc oxide nanoparticles ZnO NPs. Despite their advantages, the stability and functionality of these NPs could be impaired, and they migrate when contacting the skin, which could subsequently pose a serious hazard to human health. In this context, this study investigates the potential of using electrospun Polyvinylidene fluoride (PVDF) nanofilms incorporating by ZnO-NPs. Therefore, we investigated the migration of Zn in different simulants and its effect on the functional properties of the film. The presence of Zn in the simulants was verified by inductively coupled plasma mass spectrometry, the film was characterized by scanning electron microscopy (SEM) and infrared spectroscopy (IR), then we studied the antimicrobial activity against Staphylococcus aureus. The study shows that the antimicrobial activity of PVDF nanofilms was significantly affected by ZnO migration. Therefore, special attention should be paid to the use of these films, as Zn can probably migrate, and consequently, their antimicrobial functions may no longer be effective.

# O16. Rheological Characterization of 2D Nanoparticles Suspensions

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Graphene nanoplatelets (GNP), hexagonal boron nitride (hBN), and molybdenum disulfide ($MoS_2$) inks have recently been studied to produce electronic circuits using printing techniques [1-3]. However, there is a lack of works dealing with a complete rheological characterization of these inks. Therefore, the purpose of this work is to rheologically characterize suspensions of GNP, hBN, and $MoS_2$ with a concentration of 0.2 mg/ml dispersed in a polymeric solution of toluene and ethyl cellulose (EC) with different concentrations (0, 2.5, and 5% w/v). The shear rheological characterization was developed in a rotational shear rheometer (Anton Paar MCR 301), whereas the extensional rheology was performed by using a Capillary Breakup Extensional Rheometer (CaBER).

On one hand, steady shear experiments allowed to observe that all suspensions exhibited a slight shear thinning behavior. When the dispersion medium is pure toluene, shear-thinning occurs at low shear rates, meanwhile, for samples containing EC, this behavior was observed at higher shear rates. Moreover, the particle shape resulted in no effect on the viscosity curves. On the other hand, under extensional flow, it was verified that the suspensions without EC presented profiles of the temporal evolution of the minimum diameter similar to the profile obtained for a Newtonian fluid; for suspensions with EC, the curves obtained resembled the features of a viscoelastic fluid. In this latter case, it was found that the presence of either GPN or $MoS_2$ reduces the relaxation times of the carrier fluid to the half, whereas hBN has no effect at all. The beads-on-string phenomenon was also observed before the break of the filament at 2.5% w/v of EC and the presence of the particles had no effect at all on it.

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# O17. Rheological characterization of eco-friendly non-Brownian suspensions

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This work is framed within the project aiming at developing antivibration composites made from micro agglomerated cork pads engraved with microchannels filled with a shear thickening fluid (STF), further developing the previous studies where these composites were designed to absorb the energy of an impact load [1]. Thus, a complete rheological characterization is essential to fully understand the behaviour of the shear thickening fluid to be used.

Different environmentally friendly formulations for the STFs have been developed and tested. These formulations consisted of concentrated dispersions of non-Brownian particles of precipitated calcium carbonate (PCC) in glycerin varying mass concentrations combined with four particle aspect ratios. A full rheological characterization has been developed under simple shear (steady and oscillatory tests, i.e., SAOS and LAOS) and elongational flows [2] at different temperatures. The study allowed not only to select the most convenient particle aspect ratio and concentration of PCC, but also allowed to observe a clear viscoelastic behaviour that showed unexpectedly "*Beads On A String (BOAS)"* structures under extensional flow, which is characteristic of polymer solution [3].

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# O18. Insights on the Structural Properties of 45S5 Bioactive Nanoglasses via Molecular dynamics Simulations

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Bioactive glasses are widely employed for bone regeneration in the fields of tissue engineering and orthopedic implantation, due to the important role of the diffusion and kinetics in the ion release of this type of biomaterials, which act by inducing hydroxycarbonate apatite (HCA) to grow on their surface. In this paper, we performed molecular dynamics (MD) simulations to tackle the dynamic and structural properties of 45S5 nanoglass model through the consolidation of the amorphous nanoparticles. We find that the resulting 45S5 nanoglass consists of melt-quenched glassy cores connected by interfacial regions, the results show that these two distinct regions are well correlated with the dynamic behavior and structural features at the level of medium/ and short range order. Moreover, despite the unchanged network connectivity relative to the bulkglass, nanoglass shows an improved atoms mobility, especially sodium and calcium cations which are affected by the decreased coordination number and the increased of the atomic volume.

# O19. The application of different orientation of orthotropic composite beam

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In this paper, the dynamic analysis of orthotropic materials applied to the laminated composite beam has been studied to improve the simplification of the process of homogenizing heterogeneous composite materials [1].

This study is based on classic stratified theory of von Karman formulation and the kinetic energy of euler bernoulli developed [2] through displacement relations.

The model used in this study to explain the problem of non linear geometry in the free vibration applied of laminated beam is based on the hamilton's principle for solving the motion equation and determining the frequency of the reaction of the rolled beam.

The numerical of the symmetric an asymmetric material gives a good idea of the behaviour of the orthotropic materials, and to minimize the problem of many areas used these materials such as: dental medicine, aeronautical, aerospace, because they have a good strength, high rigidity [3].

The comparison between the different orientations may give greater importance to this study and open the search to simplify the problem of non-linear geometry and give a good result about the older other published [1].

For instance, the application of medicine, the researcher has to decode the compatibility of the human body with new materials, and to minimize the problem of deterioration [4-5].

All time the materials are evolved for new applications and reveal a lot of new problems. Therefore, the composite materials is a good role in life and in future [6-7].

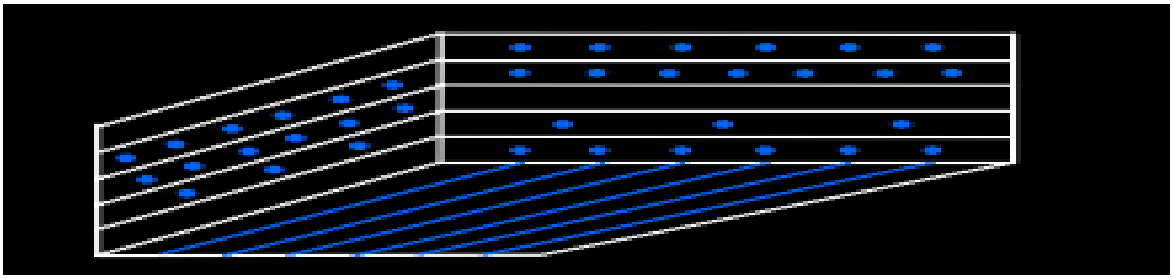

Figure 1. laminated composite beam.

| $W_{max}$(cross ply symmetric) | Wnonlinear | $W_{max}$(cross ply asymmetric) | Wnonlinear | $W_{max}$(woven) | Wnonlinear |
|---|---|---|---|---|---|
| 0,24 | 1,01 | 0,24 | 1,009 | 0,237 | 1,05 |
| 0,32 | 1,017 | 0,3 | 1,016 | 0,316 | 1,087 |
| 0,4 | 1,028 | 0,39 | 1,026 | 0,39 | 1,13 |
| 0,5 | 1,04 | 0,47 | 1,03 | 0,47 | 1,18 |
| 0,554 | 1,054 | 0,55 | 1,05 | 0,54 | 1,24 |
| 0,6 | 1,07 | 0,63 | 1,06 | 0,62 | 1,30 |
| 0,7 | 1,09 | 0,71 | 1,08 | 0,7 | 1,37 |
| 0,8 | 1,1 | 0,78 | 1,09 | 0,774 | 1,44 |
| 0,88 | 1,12 | 0,86 | 1,11 | 0,85 | 1,5 |
| 0,944 | 1,15 | 0,94 | 1,14 | 0,922 | 1,59 |

Table 1. Comparison between cross ply symmetric and asymmetric and woven.

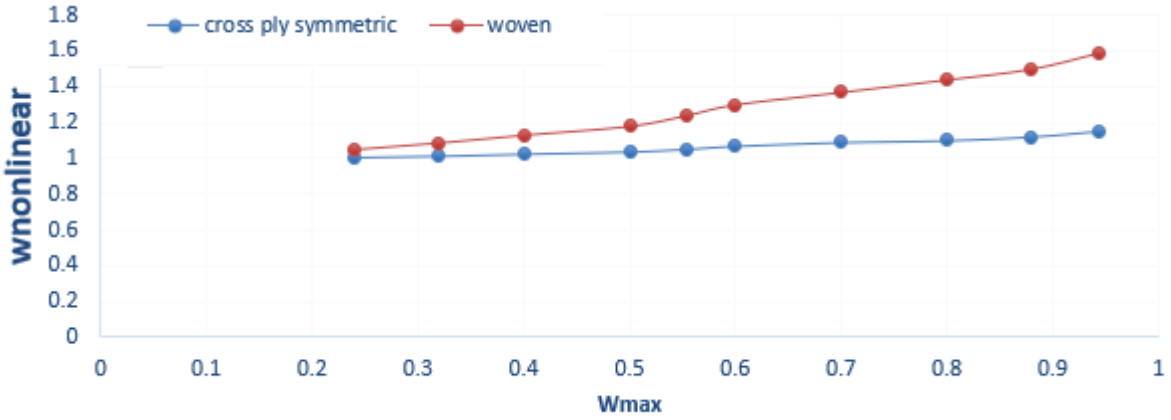


Figure 2. Comparison between cross ply and woven.

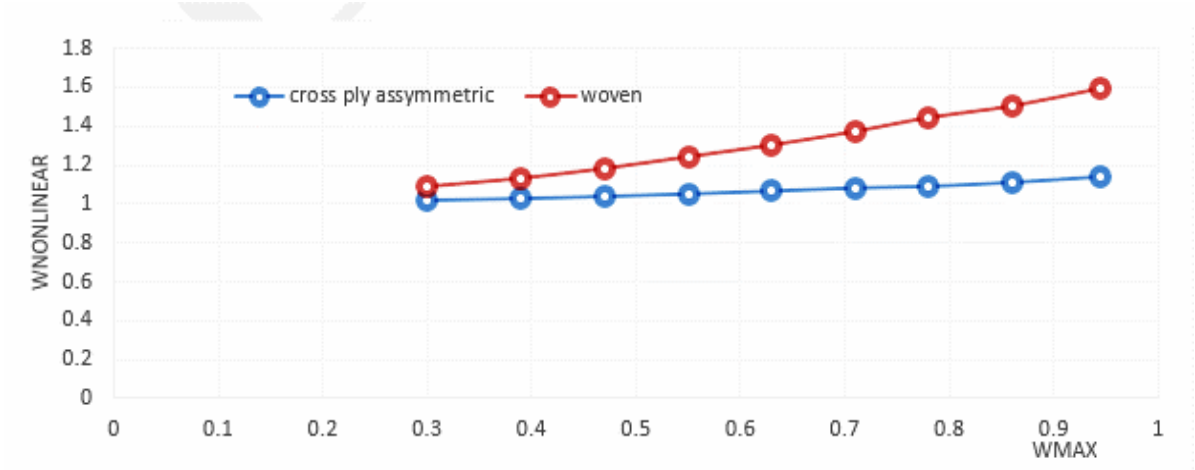


Figure 3. Comparison between cross ply asymmetric and woven.

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# O20. Double two-photon absorption in a asymmetric stepped quantum well in the terahertz range

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The electronic states are calculated for the asymmetric AlGaAs/GaAs stepped quantum well. The results show a singular behavior of the energy levels as a function of the step layer's width $Lw_2$. Indeed, we show the existence of plateaus laying within certain $Lw_2$ intervals. Added to the broken selection rules, this offers more frequency modulation of the intersubband transitions. As a major consequence, there is at least one crossing between two different transitions that occurs for many geometries (at specific $Lw_2$ widths), which may enhance the optical properties (absorption and emission) in unipolar based devices. We have, then, performed the calculation of the optical absorption coefficient, in order to evaluate the response of such specific structures to an electromagnetic radiation, especially in the terahertz (THz) domain. The calculations are performed for a particular structure where a double two-photon absorption (TPA) may occur. The first TPA corresponds to the $E_{12}$ and $E_{24}$ transitions crossing at 70meV (17THz) and the second to the crossing of $E_{23}$ and $E_{34}$ transitions at 35meV (8.5THz).

# O21. Computational insight into thermal and vibrational properties of the fresnoite and the barium titanosilicate glasses

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The Fresnoite ($Ba_2TiSi_2O_8$) (BTS) provides useful properties such as ferroelectricity, piezoelectricity, surface acoustic waves, and optical nonlinearity due to presence of unusual five-coordinate square-pyramidal $TiO_5$ polyhedral and $Si_2O_7$ groups forming two dimensional linkages [1-2]. In the other hand they can easily be obtained as polycrystalline but polar materials and that's offer the possibility to produce piezoelectric devices applicable at high frequencies who's can be used as acceleration sensors, e.g., as an air bag sensor in automotive or energy harvesting were frequent movements. Another application is in the immobilization of short-lived fission products in radioactive waste [3]. In our work we study the thermal and vibrational properties of fresnoite crystallin as for the glass and glass-ceramics using molecular dynamics simulation which give as a new insight into the understanding of thermal and vibrational properties of BTS, in crystal we study the thermal properties at high temperature the reason because the good thermal stability, together with the high piezoelectric properties and electrical resistivity makes the fresnoite a promising material for high temperature sensor, in this work we are studying the thermal conductivity using MD simulations with the Green-Kubo method with a range of temperature up to 900K and we also using the Allen-Feldman method for investigating the phonons types (diffusons, propagons) contribution to the thermal transport for the glass and glass-ceramics to investigate the transport behavior in the bulk as well as in the interface. For the glass our interesse is in the low temperature universal anomalies observed in glasses such as the plateau in thermal conductivity and the excess in specific heat and vibrational density of states.

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# O22. Effect of natural graphite addition on metakaolin based geopolymers: A Mechanical and Microstructural Study

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The main objective of this research is to develop a geopolymer formulation based on kaolin and reinforced with natural Moroccan graphite. A metakaolin (MK) was derived from calcined kaolinite, and the natural graphite was prepared by crushing, grinding and sieving to select the finest fraction. The geopolymer composites were synthesized through geopolymerization process. The mechanical, physical, and microstructural characteristics of geopolymer composites were evaluated in relation to the NG/MK ratio (0-0.7wt %). Many methods, including XRF, TGA, FTIR, XRD, and SEM/EDS, were employed to analyze the raw materials and phase formation, as well as the microstructure of the geopolymer composite. The mechanical parameters of the composite indicated that the optimal ratio of NG/MK is 0.3, which boosts the compressive strength by 49 % above the reference based on the mixing rule and high mechanical properties of graphite. Furthermore, we discovered that the inclusion of natural graphite (NG) increased the setting time of the geopolymer composite paste when compared to the reference matrix. At the microstructural level, SEM/EDS indicated that graphite sheets are integrated in the geopolymeric network and that the amount of carbon rises with the Gr/MK ratio while having a substantial influence on the densification of the geopolymer composites. Based on these findings, this geopolymer composite offers both economic and environmental potential in construction site.

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# O23. Synthesis and structural Characterization of Cu Substituted $SrCoO_3$ Perovskite Oxides

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In this work, $SrCo_{1-x}Cu_xO_3$ perovskite-type metal oxides (x = 0.00, 0.1, 0.2, 0.3) were prepared by sol-gel method using citric acid as chelating agent. We have focused on examining the effect of partial substitution of cobalt by copper on the phase purity and crystallinity of the end products. The samples obtained after calcination at 900°C for 6h were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (IRTF) and powder size distribution (PSD). XRD patterns indicate that a stable perovskite phase with rhombohedral system has been obtained for all the compositions with no detectable secondary phase where the crystallite size ranges from 48.74 to 53.49 nm. The crystallite size decreases with increasing the copper amount. The grain size of oxides as determined from laser diffraction ranges from 0.13 to 0.156 micron, this result reveals that agglomerates are present in the suspension. Infrared spectroscopy shows a broad characteristic band of absorption observed around 581 $cm^{-1}$ was attributed to the BO (Co-O, Cu-O) stretching vibration. This band is characteristic of the perovskite structure $ABO_3$.

# O24. The study of Benzene adsorption on clean and doped Ag (100) surfaces using DFT

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Using density-functional theory, we investigate the adsorption of benzene on silver (100) doped with Au, Pt, and Pd atoms (DFT). By comparing the results to the PBE calculation, we analyze the influence of the optimized vdW-DF (optB86-vdW[1]) approach and the doping effect on adsorption. The estimated findings show that when Benzene is doped with Pd or Pt atoms, its interaction with the surface steadily rises. The adsorption energies obtained increases in the order 4Au-Ag (100) < Ag (100) < 4Pd-Ag (100) < 2Pt2Pd-Ag (100) < 4Pt-Ag (100).
The Bader analysis shows that the charge transfer occurs from the molecule to the clean and doped surfaces with Au and Pt atoms and from the surface doped with Pd to the molecule.

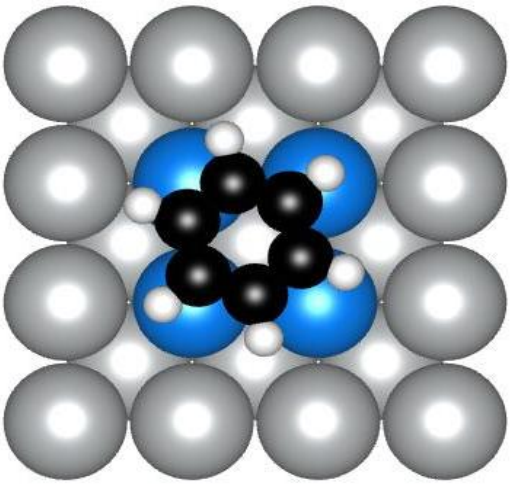

**Figure 1 : Top view of the hollow configuration of benzene molecule on doped Ag (100) surface by Pt tetramer**

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# O25. Wear Resistance of Recycled Polyamide Powder PA 3200 GF Produced by SLS

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Additive manufacturing methods have started to be widely used in our daily life by enabling the production of complex geometry materials with precise tolerances. Selective Laser Sintering (SLS) production system, which offers additive manufacturing capability for the use of this method in industrial applications, alternative material production was preferred with. For this reason, to adapt the SLS system to the test samples, recycled PA 3200 GF powders were produced in 30x30x10 $mm^3$ dimensions to form a layer thickness of 100 µm. In addition to the comparison of the mechanical properties of the produced samples, solid particle erosion wear experiments, in which the erosive particle contact under impact is important, were carried out in accordance with ASTM G76-95 standard. In the experiments carried out, the effects of the impact velocity variability (1, 2, 3 bar) on different printing directions were investigated by keeping the erosive particle size constant at four different values of the impact angle. As a result, the response of different printing direction to erosive particles differed, and the printing direction showed a significant variability in erosion resistance as well as the impact angle.

# O26. Exploring the Ti influence on the electrochemical reduction of iron from iron oxide based ceramics

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The electrochemical reduction of iron oxides to iron in alkaline media represents a $CO_2$-lean novel approach for iron making compared to the conventional carbothermal reduction process [1]. Iron oxides ores are frequently used as feedstock materials due to their abundance and low cost. Iron-bearing minerals, such as pseudobrookite ($Fe_2TiO_5$) are an interesting feedstock for this purpose. The present work explores the Ti-effect during the electroreduction to Fe imposed by highly-porous $Fe_2TiO_5$ ceramics as an alternative raw material. Hematite and $Fe_2O_3$-$Fe_2TiO_5$ composite cathodes were prepared for the sake of comparison. All highly-porous cathodes were processed based on powder water suspensions followed by emulsification with liquid paraffin, as described in [2]. The electrochemical tests were performed in alkaline conditions (NaOH, 10 M) at 80 °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 (-1.30 to -1.15 V, 7 h) and cyclic-voltammetry (-1.2 to 0 V, 10 mV/s) studies. Combined XRD/SEM/EDS studies revealed the Fe formation only at -1.30 V, indicating a compromise of the current efficiency due to strong hydrogen evolution. Despite the presence of Ti as a non-conductive phase imposed complex effects during the electroreduction, one can still take into consideration the obtained material for catalysis applications and/or consider the iron enrichment of Ti-containing iron oxide ores for further electroreduction.

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# O27. Vanadium (oxy)nitride as a potential anode for ammonia solid oxide fuel cells

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Ammonia ($NH_3$) is considered as a potential energy carrier to be used as a fuel in energy conversion devices [1], such as solid oxide fuel cells (SOFCs). These eco-friendly systems can directly convert chemical energy into electricity [2]. Nevertheless, a challenge still remains for finding alternative anode materials, aiming to improve the durability/stability and the performance of the cell components [3]. Hence, in the present work, we propose a novel candidate as electronic conducting phase, made of vanadium (oxy)nitride (VON). This interstitial alloy has been proved to be a good catalyst for ammonia decomposition and to possess excellent electrical conductivity having similar properties to the platinum group metals.
The present work is, thus, dedicated to the synthesis and electrochemical characterization of a novel cermet-based composition made from this VON phase and an oxide-ion conducting phase, $(ZrO_2)_{0.92}(Y_2O_3)_{0.08}$ (8YSZ). X-ray diffraction (XRD) revealed that cubic rock-salt structure of VON was successfully synthesized by the ammonolysis route and the compatibility tests showed no chemical interaction with 8YSZ at 1150 °C in reducing conditions. The electrochemical impedance measurements (EIS) show that the peak performing composition is that of 50:50 % volume of VON:YSZ. The electrode mechanism is outlined for the first time in an ammonia atmosphere, being similar to that of Ni-based cermets using hydrogen fuel.

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# O28. $SrTiO_3$-based thermoelectric fibres grown using Laser Floating Zone processing

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Thermoelectric technology has great potential to contribute to the challenge of recovering waste heat if efficient, cheap and environmentally friendly thermoelectric materials are developed [1]. Semiconducting oxides [2] with appropriate electrical and thermal transport properties, based on abundant, mostly non-toxic elements, in opposition to traditional thermoelectrics, show great promises for the conversion of waste heat from nuclear stations, thermal power plants, combustion engines and exhaust gases of high-temperature industries [1]. $SrTiO_3$ is a promising TE oxide, as confirmed by the previous TE studies of $SrTiO_3$ single crystals [3,4]. Undoped $SrTiO_3$ is an insulator with no free electrons, but when doped with a rare earth element like La or a transition metal like Nb, it becomes an n-type semiconductor with metallic behaviour [5]. Electron-doped $SrTiO_3$ has a large ZT not only because of its relatively high electrical conductivity but also a high Seebeck coefficient promoted by high carrier mobility and large effective mass [3]. In this work, the Laser Floating Zone method was employed for the first time for processing thermoelectric $SrTiO_3$-based materials, taking advantage of promising performance achieved for laser-processed manganites [6]. The grown fibers present good mechanical strength, high density and high values of electrical conductivity, resulting in high thermoelectric performance. Various processing variables were considered, including different growth rates, distinct growth atmospheres and thermal post-treatment of the laser-grown samples.

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# O29. Tunning the Thermoelectric properties via Substitution and Defect Chemistry engineering by Taguchi plan

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One of the promising methods to recover the wasted energy, produced in different industries or natural processes is “green” thermoelectric power generation. Nowadays particular interest is given to the oxide materials, due to have good thermoelectric properties specially at high temperature, as well as absence of toxicity, and natural abundance of prospective constituent compounds. In this work, focus is on one of the promising ceramic n-type materials with the perovskite structure, i.e., $BaTiO_3$, through solid state technique. Microstructural and chemical engineering approached, among other, on different atomic sites of these materials prove to be an effective method to enhance their thermoelectric properties. Therefore, this work will explore the effects of modification on A and/or B sites.

In order to reduce the total number of experiments, Taguchi planning with three variable parameters, three levels, were selected to evaluate the effects of substitution of Ta in B-site, deficiency of Ba in A-site, with general $Ba_{(1-x)}$ $Ti_{(1-y)}$ $Ta_yO_3$ (where x= 0, 0.025 and 0.05 and y= 0, 0.05 and 0.1) formula, and synthesis temperature. Phase identification was performed through powder X-Ray Diffraction (XRD) analysis, for all samples at room temperature. Morphological and microstructural characterization of fractured samples was performed using scanning electron microscopy complemented by energy-dispersive spectrometry for elemental analysis. Electrical conductivity and Seebeck coefficient values were measured simultaneously using the four-point probe method in home-made apparatus.

According to the Taguchi results and considering the correlation matrix and fitting parameters (see table) the substitution of Ti with Ta is the only parameter that has a pronounced effect (and in a right direction) on the electrical properties.

| Property | Correlation matrix | | | Fitting parameters | | | |
|---|---|---|---|---|---|---|---|
| | $Y_{Ta}$ | X | $T_s$ | α | β | γ | Θ |
| **Conductivity (400)** | 0.849 | -0.005 | 0.286 | 372.61±37.26 | -4.505±0.23 | 169.94±12.58 | -9.9 |
| **Conductivity (800)** | 0.913 | 0.081 | 0.165 | 320.4±32.04 | 56.62±2.83 | 78.42±5.80 | -6.75 |
| **Seebeck (400)** | 0.813 | 0.273 | 0.203 | 3163±316.27 | 2122±106.09 | 1067±78.93 | -557.8 |
| **Seebeck (800)** | 0.707 | 0.292 | 0.199 | 2802±280.21 | 2317±115.83 | 1067±78.94 | -604.4 |
| **PF (400)** | 0.773 | 0.027 | 0.412 | 1.279±0.13 | 0.088 | 0.921±0.07 | -0.041 |
| **PF (800)** | 0.860 | 0.082 | 0.285 | 2.046±0.2 | 0.391±0.02 | 0.916±0.07 | -0.046 |
| **Density** | 0.089 | 0.039 | 0.383 | 1.133±0.11 | 1±0.05 | 6.577±0.49 | 4.816 |

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# O30. Impact of the substrate composition to the deposition process of the iron from highly alkaline suspensions

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Despite the rising demand for new materials, such as aluminium, plastics and carbon composites, iron and steel, plays a crucial role in the modern world. Though, the iron industry is one of the most CO2 producers in the modern world. Also, the production of iron requires a significant amount of carbon, which can be a problem in near future considering rising prices for fossil fuels. Therefore, breakthrough technologies are urgent and indispensable. One of the possible methods that can be used in future is the electrochemical deposition of the iron from oxide suspensions [1-2]. This method allows not only significantly decreases the amount of greenhouse gassed emissions, but also can be easily used in collaboration with renewable energy sources with flexible prices in different periods.

In the current work, we will present the influence of the substrate composition on the deposition process of the iron from highly alkaline suspensions. It was found that depending on the substrate material the potential or current during deposition can significantly differ in galvanostatic or potentiostatic mode respectively. Deposition of carbon substrates, namely graphite and glassy carbon has shown the least efficiency. At the same time, deposition nickel shows a current density up to two times higher. Deposition behaviour and comparison of the deposit properties will be discussed in the presentation. Feasibility and possible interests in industrial applications will be also discussed.

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# O31. Prospects of iron electrowinning from an iron-rich industrial residue

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The development of energy-efficient, carbon-free, and environmentally friendly routes to produce iron and steel is critical. Direct electrochemical reduction of iron oxides has been gaining attention as a process allowing in-situ reductions at the cathode, under strong alkaline media with hydrogen and oxygen as by-products. This technology also considers the integration of renewable energies and reduces 87% of the direct $CO_2$ emissions [1–2]. In this scope, the present work consists of the novel electrochemical reduction of akaganeite (β-FeOOH) particle suspension into iron, under a strongly alkaline solution at low temperature, to study the prospects of using a metallurgical waste as an iron oxide source in comparison with the synthetic composition. The by-product of nickel manufacture is also studied in the frame of this work. The synthetic β-FeOOH and the industrial residue depositions were performed in 10 M of NaOH as electrolyte at moderate temperatures of 90 ºC. The deposition was performed in both galvanostatic and potentiostatic conditions. This allowed optimizing the microstructural composition of the iron. The selected experimental conditions allow efficient deposition of the iron without significant evolution of hydrogen, allowing an efficiency increase in comparison to the deposition from dissolved iron salts or conventional acidic suspensions. Cyclic-voltammetry was used to characterize the deposits from the electrochemical point of view. Combined studies of XRD/SEM/EDS proved the presence of Fe crystals with this electrochemical system. Certain differences in iron microstructure were found. It is shown that relatively high efficiencies can be achieved in both synthetic akageneite and industrial sludge.

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# O32. Detection of Bile acids using Optical Biosensors based on Cholesteric Liquid Crystal Droplets

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We report a novel highly sensitive bile acids (Cholic Acid & Deoxy Cholic Acid) biosensor based on PVA/SC12S stabilized cholesteric liquid crystal droplets. These CLC droplets are monodisperse in nature and are generated by fabricating the capillary microfluidic flow focusing device. Homeotropic to planar transition of CLC droplets would be triggered during a competitive adsorption of bile acids at the surface of CLC droplets. This sensor detects bile acids at a minimal cost, in a simple and quick manner. The detection limit of our method for CA is (1 µM) 80% lower and for DCA is 50% lower than previously reported by using nematic droplets for the detection. Furthermore, the response times and detection limits of these bile acids, can be adjusted as a function of pH, bile acid volume, and droplet size. Bile acids can be identified without the use of crossed polarizers using this novel method.

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# O33. $Ba_2NiMoO_{6-\delta}$ as a potential electrode for protonic ceramic fuel cells at intermediate temperature (400-600°C).

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Perovskite related materials exhibit several fundamentally interesting chemical and physical properties, which can be combined in a single material, and where these properties can be refined for application as possible electrode materials by compositional modification [1]. For example, their structural and compositional flexibility can allow partial cation substitution on the A or B sites, giving rise to a subclass of the perovskite family, commonly designated as double perovskites ($A_2BB'X_6$) [2]. Double perovskites are gaining special interest as electrocatalysts, due to their good chemical stability, high eletronic conductvity and high electrocatalytic activity for the oxygen evolution, oxygen reduction and hydrogen evolution reactions [3].

In this work we investigate the use of the layered double perovskite $Ba_2NiMoO_{6-\delta}$ (BNMO) as a potential electrode for protonic ceramic fuel cells in the intermediate temperature range (400-600°C). Studies of chemical stability and compatibility, as well electrochemical performance were performed as function of composition, by varying the compositional ratio of $BaCe_{0.7}Zr_{0.1}Y_{0.2}O_{3-\delta}$(BCZY712)-BNMO in composite electrodes.

To understand the electrochemical behaviour of BNMO and BNMO-BCZY composites, symmetrical cells were prepared and tested, where the electrode materials were deposited on BCZY712 electrolytes by screen printing method and studied using electrochemical impedance spectroscopy in wet $O_2$ ($pH_2O$=0.03 atm) in the temperature range 600-400°C. Results reveal that the BNMO-BCZY712 composites can exhibit good electrochemical performance, with the best behaviour offered by the 40vol% BNMO-BZY712 composite composition.

To the best of our knowledge this is the first study of the layered BNMO double perovskite for proton conducting applications. Continued work aims to further improve these electrodes by control of electrode thickness and processing parameters.

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# O34. Hyaluronic acid packed in transethosomes for topical delivery

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Hyaluronic acid (HA) has a key role in tissue regeneration and effective anti-ageing due to its properties like skin hydration, wound healing, and UV radiation-protective ability.[1] Decreased amounts of HA in ageing skin are associated with loss of skin moisture.[2] The skin penetration of HA is limited by low permeability and large molecular size.[3] Hence, we decided to encapsulate HA in transethosomes (TEs), which are nanocarriers with ultra-deformability and enhanced skin permeability properties, to improve its skin delivery. TEs composed of egg yolk phosphatidyl-choline and surface-active agents (jojoba oil or tween 80) containing HA of two molecular weights (20-60 kDa and 650 kDa) were prepared by the thin-film hydration method with following sonication. The nanoparticles were characterized by dynamic light scattering (DLS), scanning electron microscopy (SEM) and high-performance liquid chromatography (HPLC) with a UV detector. Produced HA-loaded transethosomes showed storage stability up to 10 weeks and more than 87% HA inclusion in the TEs. The polydispersity index (PDI) is slightly higher than 0.2, which indicates an almost homogenous population of TEs. Zeta potential values verified the stability of formulations. Stable delivery systems containing HA were produced. Most of the studied formulations show high loading capacity and good potential for skin application.

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# O35. Synthesis of ambient pressure–dried hydrophobic silica aerogel

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Aerogels which are synthesized via sol-gel method contain nanopores in their structure. Aerogels are filled with air by 90-99% by volume. As a subclass of aerogels, silica aerogels have unusual features such as low density, high specific surface area, high porosity and low thermal conductivity [1]. Thanks to these thermal and structural properties silica aerogels are useful as adsorbent of dyes [2], carrier in drug delivery systems [3], hydrogen production [4], thermal insulator [5], cement raw material as an alternative to sand [6]. Because silica aerogels possess OH groups, their surface can be damaged easily under humid conditions. To overcome this undesired situation, researchers have utilized several surface modification agents such as trimethylchlorosilane (TMCS), hexamethyldisilazane (HMDZ) in the silica aerogel synthesis [7]. In the case of drying at ambient pressure, cheap sodium silicate source has been generally used. But this process requires extra expensive chemicals such as cationic resins. The purpose of this study was synthesis hydrophobic silica aerogel at ambient pressure via feasible two step acid-base sol-gel method by using common TEOS precursor. Synthesized silica aerogel was characterized by using XRD, TG/DTG/DTA and FTIR.

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# O36. Novel application of plasma treatment of polymer and composite powders for 3D additive manufacturing

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This is a comprehensive research study on the use of plasma treatment as an emerging method for the preparation of laser sintering powders aiming to address the laser sintering challenges and improving the properties of the end-use parts.

Plasma-assisted surface modification are carried out on two different types of nanoclays to prepare polyamide 12 (PA12) nanocomposites for applications laser sintering (LS). A reduction of the rounded aggregates of the nanoclay particles and improvement of the thermal stability of two different nanoclays (C30B and I.34TCN) were achieved due to plasma treatment as indicated by SEM micrographs and TGA analysis coupled with the FTIR spectra. Some mechanical properties demonstrate an improvement when including plasma-treated nanoclays (over non-treated and pure Polyamide12).

The second part of this project includes an attempt to suggest uncommon using of plasma for treating Laser Sintering (LS) polymer powders with the aim of improving the adhesion and wettability for user-friendly biomedical applications. The targeted material polyamide 12 (PA12) was exposed to air plasma treatment for different time durations: 1-3 hours. An increase the crystallinity accompanying with the density increase and removal of amorphous components and improve the powder wettability due to the surface functionalization during the plasma exposure were obtained.

Our previous works displayed the feasibility of using the treated C30B with polyamide 12 in downward heat sintering method (DHS) [1-2], and the usability of treated I.34TCN with the polyamide 12 in laser sintering (LS) applications where DHS was used to set LS parameters [3]. In addition, our attempt on plasma treatment of PA12 has led to morphological and chemical changes resulting in porous particles with higher hydrophilicity than nontreated PA12 [4-5]. Besides the usefulness of this approach for producing wettable and high crystalline powder made by treated PA12, testing the LS parts produced by the treated powders is required in future work.

Finally, it can be concluded that the air plasma treatment of clays has demonstrated to be successful tool for the preparation the polymer nanocomposite for laser sintering.

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# O37. Solid waste recycling in alumina technical ceramics production

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Alumina powder is categorized as inert and non-toxic, which means that it can be safely reused after machining a green body. The green body is usually obtained in advanced ceramic manufacturing by compacting raw alumina powder into a rigid shape using applied pressure. The possibility of reusing generated alumina solid waste as secondary raw material has been investigated. The alumina samples were formed by slip casting, which utilizes an aqueous slip of commercial alumina powder mixed with 20 dwb. % of alumina waste powder (expressed on a dry weight basis) and porous mould. The prepared alumina samples were characterized and successfully sintered. The applied sintering methods were one-step and hybrid microwave sintering methods. Finally, alumina samples without the addition of waste alumina powder were also sintered to compare two sets of samples. The sintered samples with the addition of alumina waste powder showed higher theoretical density, which reflected onto slightly better mechanical properties such as indentation fracture toughness and Vickers hardness. The better mechanical properties of ceramic samples containing waste alumina are a consequence of lower porosity due to a higher amount of magnesium oxide present in alumina waste powder. The conducted research strongly suggests the possibility of reusing waste alumina powder in advanced ceramics manufacturing.

# O38. Physical and electrochromic properties of Prussian Blue thin films prepared under different electrodeposion times on ITO substrates

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A set of Prussian Blue (PB) thin films were prepared with different electrodeposition times [1]. The films were characterized by a variety of physical methods (such as X-ray diffraction, field effect scanning electron microscopy, Fourier transform infrared spectroscopy and UV-Vis spectrophotometry), and electrochemical techniques. A simple and established electrochemical method was used to estimate the optimal voltages for coloring and bleaching of the different PB films. Controlling the electrodeposition time, along with the application of suitable electric voltages, enabled us to investigate and improve the electrochromic properties of the PB films.

The results show that the sample prepared with 75 s deposition time exhibits good electrochromic response [2,3], a high value of electrochromic contrast (55.36% at 555 nm), and a good stability of ion exchange after cycling. The control of the deposition time resulted in nearly 9.4 times increase of the contrast ratio and of the corresponding value for the optical density (ΔOD) of the PB films [3]. The influence of the deposition time, structure and morphology on the electrochromic properties of the films will be discussed and presented.

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# O39. Water Pollution control & Hydrogen Production using 2D-Photocatalyst: 6, 13- Pentacenequinone (PQ)

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$Fe_2O_3$ nanoparticles of different sizes ranging from 22 to 56nm were synthesized chemically by a modified sol-gel method. Pure alpha phase particles as well as particles with admixture of alpha and gamma phase were obtained and identified by x-ray and Mössbauer measurements. Different size and phase controlling parameters have been identified. The average size of the particles decreases with increased annealing temperature of the gel and decreases with the increase in the concentrations of the (citric acid). The annealing temperature affects the relative fractions of the two phases and consequently the magnetization of the particles.

The samples were then characterized X-ray diffraction (XRD) and) Fourier transform infrared spectroscopy (FTIR) and UV-Vis spectrophotometer. XRD pattern showed that the iron oxide nanoparticles exhibited alpha-$Fe_2O_3$ (hematite) structure in nanocrystals. The α- $Fe_2O_3$ nano-powders with uniform size were prepared when the samples calcined at 500 °C, and the lowest particle size was found to be 30 nm by XRD technique The sharp peaks in FTIR spectrum determined the purity of $Fe_2O_3$ nanoparticles and absorbance peak of UV-Vis spectrum showed the small bandgap energy of 2.58 ev.

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# O40. Driving the photocatalytic activity of Fe2O3 towards TiO2 for Safranin & Rhodamine dye degradation

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Iron oxide plays important role in current industry due to its special characteristics such as anti-corrosion, anti-bacteria, has low electron conductivity and excellent heat resistance. Therefore, the objective of these study is to synthesize zinc oxide nanostructure with the most particle ways by using sol gel method and characterize the nanostructure. Sol-gel autocombustion method is the simplest method and has ability to control the particle average size less than 50nm and morphology through systematic monitoring of reaction parameters. Fe2O3 nanoparticle were synthesized via sol gel method using Fe(NO3)3.9H2O as a precursor and the water was used as a solvent, ammonia and distilled water were used as a medium. Fe2O3 nanoparticle were characterised by XRD, FESEM, and nanoparticle analyser. XRD results spectrum display mainly oxygen and iron peaks, which indicate the crystallinity in nature as exhibiters. FESEM micrographs shows that synthesized Fe2O3 has rhombohedral structure. The obtained Fe2O3 particle are homogenous and consist in size which corresponds to the XRD results that exhibit good crystallinity. This paper demonstrates the synthesis of Fe2O3 nanoparticle using a sol gel auto combustion method using ferric nitrate and citric acid in solvent medium water. 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, concluding the higher degradation rate for high % TiO2 than lower. The proposed method can also be used for synthesizing other semiconductor TiO2 containing nanoparticle.

# O41. Novel $AgFe_2O_3$-PQ Composite for the Photocatalytic Application

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Silver iron oxide plays important role in current industry due to its special characteristics such as anti-corrosion, anti-bacteria, has low electron conductivity and excellent heat resistance. Therefore, the objective of these study is to synthesize Silver iron oxide nanostructure with the most particle ways by using sol gel -autocombution method and characterize the nanostructure. Sol-gel method is the simplest method and has ability to control the particle size and morphology through systematic monitoring of reaction parameters. $AgFe_2O_3$ nanoparticle were synthesized via sol gel- autocombution method using silver as a precursor and the water was used as a solvent, distilled water were used as a medium. $AgFe_2O_3$ nanoparticle were characterised by XRD, UV-Visible, FTIR, FESEM, and nanoparticle analyzer. Result of XRD charactrisation shows that the $AgFe_2O_3$ nanoparticle has good crystaline structure. XRD results spectrum display mainly silver and iron and oxygen picks, which indicate the crystallinity in nature as exhibited. FESEM micrographs shows that synthesized $AgFe_2O_3$ has rod-like structure.The obtained $AgFe_2O_3$ particle are homogenous and consist in size which corresponds to the XRD results that exihibit good crystallinity. $AgFe_2O_3$ nanoparticle were successfully synthesized by sol gel autocombution method in nano size range within 81.28 nm to 84.98nm. This work demonstrates the synthesis of $AgFe_2O_3$ nanoparticle using a sol gel autocombution method. 6,13 pentacenequinone using cyclohexanedine and ortho-pthaldehyde as substrate. 6,13 pentacenequienone and $AgFe_2O_3$have band gap of ~2.5ev and 1.88ev respectively and thermal stability and photo catalytic activity. Crystal violet dye is degraded at higher rate using coupled semiconductor PQ/$AgFe_2O_3$ than individual PQ and $AgFe_2O_3$, concluding the higher degradation rate for high % PQ than lower.

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# O42. Effect of HTC doping on the performance of carbon felt as anodic electrode in microbial fuel cells

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In this work, the use of deactivated and activated HTC, obtained from *Spergularia rubra*, was studied as doping agent in carbon felt (CF) anodes used in microbial fuel cells. The hydrothermal carbonization process was carried out at 200ºC for 2 h with a biomass/water ratio of 100 g/L. In order to activate the HTC, a thermal activation at 1000 ºC was carried out in inert atmosphere, $N_2$ flow rate of 0.5 L/min. The performance of the three electrodes studied: CF, CF+$HTC_{deactivated}$ and CF+$HTC_{activated}$ are presented in Figure 1.

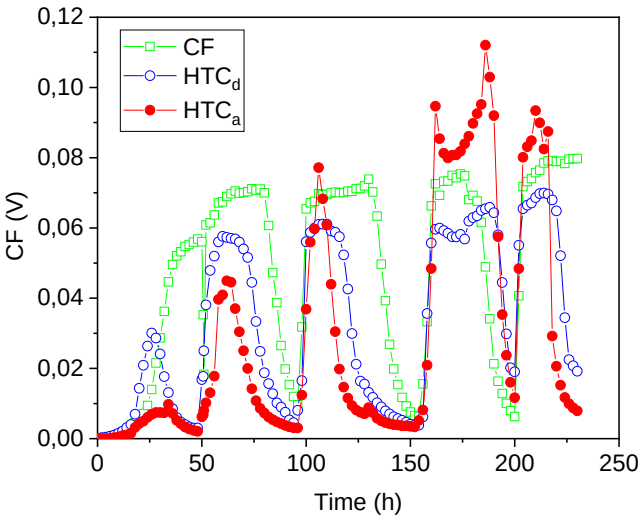


*Figure 1. Voltage generation along the time.*

From Figure 1, it can be seen that, initially, the best performance was obtained with the CF electrode. During the first hours, the deactivated and activated HTC dopped electrodes presented a poor performance, however, their performance drastically increased with the time. In the case of the $HTC_d$, after 250 h a similar performance of the CF was obtained. In the case of the $HTC_a$ after about 100 h of operation its voltage was the highest, generating 0.11 V.

From the results presented in this work, it can be concluded that the CF electrodes dopped with activated HTC presented a better electrical performance than the raw ones. This is very important because it would allow to a better energy recovery in the microbial fuel cells at the same time that a material valorization of the *Spergularia rubra* biomass can be carried out.

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# O43. Electro – Optical Performance of Coumarin dye doped Cholesteric liquid crystals for the Application of Electrically Switchable Smart Window

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In this article, bi-stable cholesteric liquid crystal (CLC) smart window has been fabricated and the effect of coumarin dye on their structural and electro-optical properties was studied. A 0.3 wt% coumarin dye was added to pure CLCs of reflecting IR, Blue. The morphological behavior of bistable CLC smart window observed to exhibit three modes represents planar (P), focal-conic (FC) and Homeotropic (H) states on applied voltages at low frequency (1KHz) respectively. The voltage-transmission characteristics were examined and found the operating voltage lowered with the doping of coumarin dye in CLC. Moreover, dye doped CLCs smart window showed three states compared with pure CLC and coumarin dye. In addition, phase transition studies of pure and dye doped CLCs have been discussed. Further, by utilizing the features we have tried to implement in authenticated/unauthenticated QR codes, smart windows, light shutters.

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# Poster presentations

# P1. Conductivity and transmittance enhancement of PEDOT:PSS thin films by graphene addition

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Compared to conventional inorganic semiconductors, organic semiconductors present several advantages, such as, cost-effectiveness, mechanical toughness, synthesis versatility and simple production set-ups, among others. In this work, we have prepared conductive solid films and trails based on multilayer graphene (mG) and poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) from liquid dispersions. mG-10.6 wt% dispersion in isopropanol was prepared in two steps. In the first step, graphite was submitted to liquid phase exfoliation in N-methyl-pyrrolidone (NMP) (5.3 wt% of mG) [1], then, in the following step, NMP was removed by precipitation and resuspension of mG, using polyethyleneimine and acetic acid-1M in isopropanol, respectively [2]. The nanocomposite films were prepared by spin coating from dispersions of mG and PEDOT:PSS to reach pre-established solid concentrations of 10.3 wt% and 50.3 wt% of mG. The optical and electrical properties of the thin films were characterized using UV-Visible Spectroscopy and an adapted four-probe resistance measurement, while Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM) were applied to analyze their morphological features. The thin films showed high transmittances, even multilayer, upholding more than 85% for three-layer films, similar to that found in single-layer ones. The sheet resistances of the films were detected in the range of a few hundreds of Ω/□. Both transmittance and sheet resistance of the films were improved when compared to those found in pristine mG and pristine PEDOT:PSS, which is attributed to higher charge mobility in the nanocomposite. SEM analysis showed that the films are largely homogeneous, and mG is uniformly dispersed, nevertheless the mG platelets appear to be standing up from the film (AFM). The phase image (AFM) allows the differentiation between rigid and soft regions, i.e., mG and polymer, respectively. Additionally, conductive trails were drawn using the dispersions and LEDs were added to the circuit and turned on under applied voltage, suggesting other applications for these nanocomposites. Semiconductive nanocomposites having high load of mG were successfully prepared, and their resulting electrical and optical properties make them suitable to be used, e.g., as transparent electrodes, in the fabrication of displays, lighting devices and photovoltaic materials or as multipurpose conductive inks.

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# P2. Synthesis and characterization of ZnAl new hybrid layered double hydroxide. Application to uranyl adsorption

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Due to the recent increase in demand for heavy metal resources, the ions of these metals released into the environment by the chemical industries namely; paints and coatings, mining, extractive metallurgy and other industries, are on the rise. The toxicity and non-biodegradability of heavy metal ions make them very dangerous to human health and lead to serious environmental problems [1-4]. Over the decades, various treatment processes, including membrane filtration, chemical precipitation, electrocoagulation, adsorption, and ion exchange, have been developed to decontaminate aquatic resources by removing heavy metal ions [5]. Of these treatment methods, adsorption is considered the most promising in terms of feasibility, regenerative capacity, low cost and high removal efficiency [6].

It is in this perspective that our work consists in the synthesis of a new hybrid material of the double lamellar hydroxide type and its application in the retention of the uranyl ion $UO_2^{2+}$.

Double lamellar hydroxide is synthesized by the co-precipitataion method and then intercalated with Taurinyl phosphonic acid which has been characterized using XRD, IFTR and BET methods. The adsorption capacity of the resulting material is studied in the retention of the $UO_2^{2+}$ ion, an excellent maximum yield is obtained by following the different optimal parameters. A kinetic study shows that the adsorption process is spontaneous, exothermic and follows the isotherm L with pseudo-second order kinetics.

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# P3. A hydrophobization of CNF and enhancement of mechanical properties of CNF-PHA composite

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As personal hygiene is emphasized in Covid 19 period, usage of disposable products is increasing rapidly and its waste such as waste plastics is increased also[1]. The waste plastics cause environment problems and thus, biodegradable plastics are being paid attention to solve the problems. The biodegradable plastics can be completely decomposed in soil by microorganisms and it can be a solution for the mentioned environmental issues.

PHA (polyhydroxy alkanoates) is a biodegradable thermoplastic produced biologically and is attracting attention as an eco-friendly packaging material due to its excellent processability and moisture barrier property. However, it is difficult to use alone due to its poor thermal and physical properties, and complexation with other polymers has been studied to enhance its thermal and physical properties [2].

In this study, cellulose nano fiber (CNF), an excellent additive for plastic composite due to its high aspect ratio, was selected to reinforce the thermal and physical properties of PHA. A silylation was applied to improve dispersibility of hydrophilic CNF into hydrophobic PHA and maintain high aspect ratio of CNF.

FT-IR analysis and SEM-EDS image analysis of silylated CNF (S-CNF), and moisture contact angle measurement of S-CNF based film were performed to determine the silane group, structural analysis, and element analysis on surface and hydrophobicity of S-CNF, respectively. It was confirmed that elongation of the PHA composite with 1% of S-CNF was 305%, an increase of about 11% compared to neat PHA, showing an improvement in elongation of PHA due to the high aspect ratio of CNF. When non-silylated CNF was added to PHA, however, no change in elongation was observed, and it was confirmed that the dispersibility of CNF was improved by the silanization.

Studies on the enhancement of tensile strength and thermal stability are being conducted by adding silanized CNF, and optimizations of the silanization process and polymerization ratio are being performed to maximize the improvement of the physical properties of PHA.

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# P4. Degradation of azo-dye by Fenton and photo-Fenton using surface-functionalized polyacrylonitrile (PAN) fibre catalyst

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Nowadays, accessible clean water and energy resources are among the highest priorities for sustainable economic growth and societal wellbeing. Water scarcity is an increasing problem globally making it imperative that wastewater is treated and reused in industrial processes, for irrigation and feeding to livestock, thus saving potable water for drinking. Up till now, semiconductor catalysts are produced in the form of a powder suspended in a model solution of pollutants. Many reactors use catalysts in form of suspension where the separation and reuse of the catalyst are difficult to achieve with significant catalyst loss, efficiency, and cost-effectiveness of the process. Regarding the practical applications, immobilised catalysts are more favorable due to the continuous mode of operation and multiple times usage.

Reactive orange 16 (RO-16) is a well-known azo-dye in the environment that is not removed during wastewater treatment because of its high persistence in the aquatic solution. The aim of this work is to evaluate the removal of RO-16 using the surface-functionalised polyacrylonitrile (PAN) mesh with Fe (III). The catalyst was tested in a reactor in batch mode at a laboratory scale at different catalytic parameters. The removal of RO-16 was detected by measuring the absorbance at 254 nm and 493 nm by UV-Vis spectrophotometer. Removal of 50 mg/L of RO-16 was achieved under UV-C radiation using 125 mg/L $H_2O_2$, 6 g PAN catalyst, 25 °C, and pH 3. After five cycles of use, there was no significant difference in the activity of the catalyst.

# P5. Correlations among mechanical properties of camel hair fiber and polypropylene fiber reinforced concrete at high temperature

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Under the effect of temperature. the concrete subjected to modification of the mechanical properties (Compression and tensile strength. This paper studied the experimental correlations between splitting tensile strength and compressive strength of camel hair fiber reinforced concrete (CHFRC1) and polypropylene fiber reinforced concrete (PFRC1) about the effects of elevated temperatures. Mixtures were prepared with water to cementitious materials ratios of 0.50. Camel hair fibers content of 1 kg/m$^3$ and polypropylene fibers 0,9 kg/m$^3$. The compressive and splitting tensile properties were measured on cylindrical and prism concrete specimens of 100 mm diameter X200 mm length and 70X70X280 mm respectively at 90 days. Specimens were exposed to temperatures of 20°C 150°C ,250°C et 500°C. for a period of 1 h. Accordingly, new non-linear equations were proposed and developed for the relationship between tensile strength and compressive strength at high temperature.

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# P6. Numerical investigation of Mixed convective heat transfer in a channel in presence baffles

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The heat transfer process is encountered in different natural and industrial applications where the process involves energy. Thermal management includes reducing heat losses or enhancing heat exchange in such systems has interested the scientists for several decades. From previous works, several methods can be employed to achieve heat transfer enhancement: passive methods by the perturbation of the boundary layer using vortex generators and active methods using moving objects or modulated flows cited by [1, 2,3]. Thus, this work falls within this sphere and attempts to contribute to understanding the unsteady phenomenon by getting as close as possible to the reality of the problem.

The object is to carry out transient simulations of the aiding mixed convection in a vertical channel with baffles attached to the heated wall.The purpose of this work is to examine the efficiency of installing airfoil-shaped disturbances to improve heat transfer without dangerously increasing the pressure drop (Fig 1).

The unsteady governing equations are solved by the finite volume method using the CFD OpenFOAM® Open souce.

The flow structure for three Reynolds number values (200, 500 and 800) and $Gr = 8\times10^4$.the steady-state behaviour is evident. In this range of *Re* and for a constant Grashof number, the flow is dominated by the buoyant forces and tends to skirt the baffle then penetrate into the cavity regions. With increasing Reynolds number, inertial forces prevail and prevent the main stream flow to penetrate into the cavity. The corresponding streamlines and isotherm contours are displayed in (Fig 1).

The results demonstrated that the baffles disturbed the boundary layer and contributed to fluid mixing. The augmentation of Reynolds number to relatively high values, the disruption induces the bifurcation of the flow to the self-unsteady state regime.

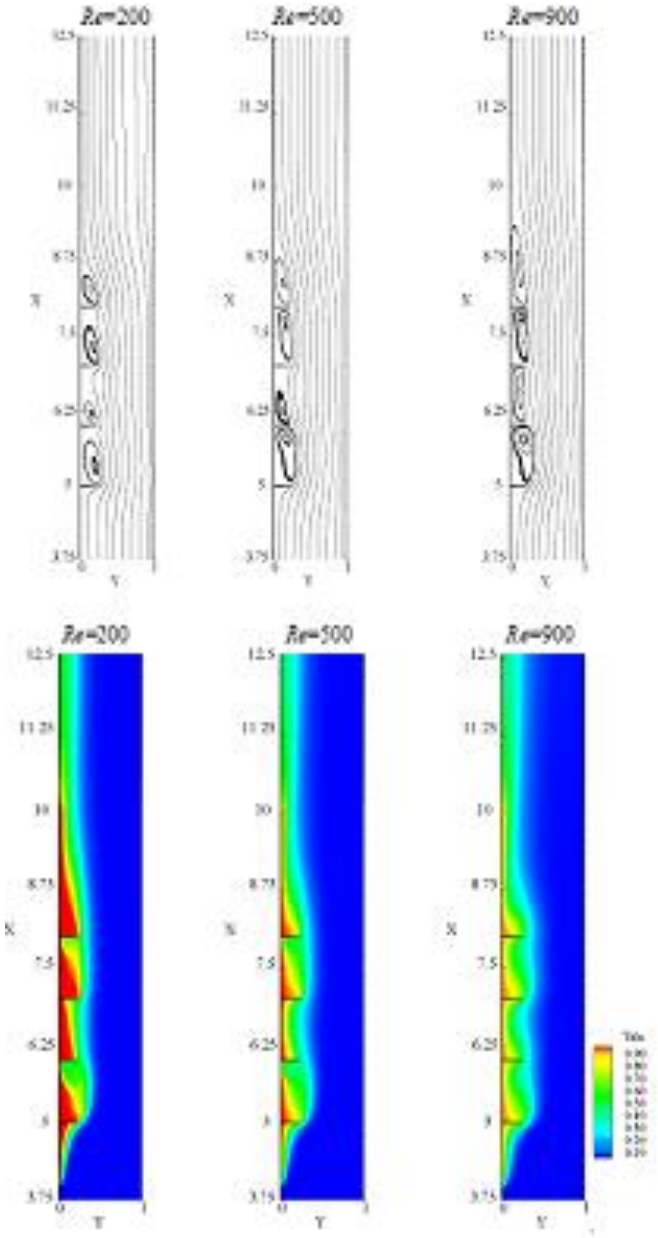


**Fig 1. Streamlines and isotherms field for various Reynolds number and *Gr* = 8 ×10$^4$.**

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# P7. Impact of Transition of Metal oxides (TiO2, MnO, CuO) On Structural, and Optical properties of Core Shell heterostructure CdS/$Zn_3(PO_4)_2$ Nanohybrid for LED applications

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Pure and Transition Metal oxide (TiO2, MnO, CuO) nanohybrid composites of CdS/$Zn_3(PO_4)_2$ synthesized by hydrothermal method at mild reaction temperature of 100°C. The prepared samples are investigated by Powder X-ray diffraction (XRD), Diffusion Reflectance spectra, FT-IR spectra, Scanning electron microscope, and Photoluminescence techniques in a systematic manner. The XRD results confirm crystalline nature of the samples with crystalline peaks corresponding to both hexagonal structure of CdS and monoclinic γ-phase of $Zn_3(PO_4)_2$. Interestingly, due to coupling of CdS with $Zn_3(PO_4)_2$, phase transition from α-Phase of $Zn_3(PO_4)_2$ to γ-phase of $Zn_3(PO_4)_2$ has been observed under hydrothermal conditions and exhibit internal structural variations due to the formation of CdS/$Zn_3(PO_4)_2$ nanohybrid. Average crystallite size, lattice strain and dislocation density are estimated by Debye-Scherrer and W-H methods. The average crystal lattice was found to be 15-25 nm. The surface morphology of the prepared samples show hexagonal spheres accumulated on rectangular flakes which indicate core-shell heterostructure. From the UV–Vis DRS spectra, energy band gap is found to be 2.42 eV that is located in the visible region and is due to quantum size effects. FT-IR spectrum shows the fundamental vibrational modes of CdS/$Zn_3(PO_4)_2$. The room temperature Photoluminescence spectra of pure and $TiO_2$ doped CdS/$Zn_3(PO_4)_2$ lattice shows a strong emission peak at ~ 518 nm in the green region, while upon the incorporation of CuO, MnO ions in host lattice, a sharp luminescence peak around 393 nm has been observed with other peaks at 494 nm, 594 nm and 684 nm which are in the violet, blue-green and red regions, respectively making them suitable for optoelectronic device applications.

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# P8. Mechanical properties of pristine and carbon nanotube poly (2, 5-benzimidazole) composite: A molecular dynamics and experimental approach.

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The mechanical properties of multi-walled carbon nanotube poly(2,5– benzimidazole), ABPBI, are explored using molecular dynamics and supported experimentally for space applications. ABPBI was synthesized and In Situ Polymerization of 3, 4-Diaminobenzoic acid with multi-walled carbon nanotube (MWCNT) was used to create the polymer composite. Molecular dynamics calculations were performed using the Materials Studio software package and the module Forcite. The resultant, simulated cells and prepared samples are illustrated in figure 1. The simulated results for ABPBI Young's modulus ranged between 2.1 and 3.8 GPa, which is in good agreement with the experimental values. When the samples in Figures 1 b) and d) were tested, the modulus for ABPBI and the ABPBI CNT composites were 1.67± 0.45 GPa and 3.22 ± 0.49 GPa respectively. This is in good agreement with results in previously published works [1] and the simulated work. Other properties compared to experimental works include densities and wide-angle diffraction patterns. The area envisioned for the polymer composite is Low Earth Orbit. In this region, temperature varies significantly. Using the molecular dynamics platform the polymer composite was subjected to this temperature range to monitor the changes in its mechanical properties.


**Figure 1: a) simulated ABPBI cell, b) ABPBI sample, c) ABPBI carbon nanotube composite simulated cell, d) ABPBI carbon nanotube composite sample**

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# P9. Novel hybrid nanofibrous membranes of Nylon 6/Yeast cell wall components for potential removal of heavy metal contaminants

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Nanofibrous membranes can be obtained by the application of high electrostatic potentials, a process known as electrospinning, showing very large surface-to-volume ratio, high porosity and interconnectivity, making them very attractive for applications like filtration, enzymatic membrane reactors, tissue engineering, sensors, or delivery matrices for bioactive and pharmaceutical compounds [1]. With the aim of obtaining nanofibrous materials with improved filtration capability and adequate performance to remove heavy metals as contaminants, for example from wastewater, we have fabricated and characterized electrospun nanofibrous membranes from nylon 6 (N6) and yeast cell wall (YCW) components. Two main biopolymeric samples were obtained by sequential extraction of yeast cell by-products with water and alkaline solutions [2]: a YCW-rich extract and a mannoprotein-rich extract (MP). Membranes of N6 alone showed satisfactory mechanical properties. SEM analysis revealed arrays of randomly distributed fibers with high porosity, and average fiber diameter of 235 nm and water contact angle (WCA) of 101°. FTIR analysis confirmed the presence of the biopolymeric components in the hybrid membranes that in general increased the membrane surface hydrophobicity. N6/YCW membranes had similar overall tensile strength properties and fiber diameters but the N6/MP membranes showed higher fiber average diameter, lower stress at break point, lower stiffness and higher elongation. Based on the potential sorption ability of yeast cell wall components [3], sorption experiments were performed for cadmium and lead cations. Promising results have been obtained and further studies are underway to better characterize the effect of initial meal ion and pH and the relative ratio of the polymeric fiber components on the sorption process.

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# P10. Corrosion protection of pipeline steels by organic inhibitors

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This paper investigates the inhibiting effect of datastone extracts (phenolic compounds) on the corrosion protection of API5LX70 steel. Corrosion resistance was evaluated, in HCL acid medium (1M), by two methods: Tests of the lost mass, without and with inhibitors, increase with the immersion time. Note that the longer the immersion time, the less corrosive the steel. This degradation of the speed can be explained by the formation of the iron oxide layer on the steel substrate in HCl medium without inhibitor and by the inhibitor effect in the HCl medium with the addition of phenolic compounds. Electrochemical polarisation measurements show that the inhibiting efficacy of phenolic compounds is 85.28%. Similar results were also found with orange peel extract. For carbon steel in HCl [1]. On the other hand, they used oleogum resim extract of ferula.assa - foetida and dorema ammoniacum for steel in HCl medium [2]. Scanning electron microscope (SEM) analysis shows the influence of the inhibitor (phenolic compounds) on pitting corrosion of API5L X70 steel in HCl medium (1M). Clearly the existence of the inhibitor, the bites have progressively disappeared.

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Table1 : Inhibitrice effecacy with immersion time.

| Immersion time (Days) | 7 | 14 | 21 | 30 |
|---|---|---|---|---|
| Inhibitrice effecacy | 79,298989 | 76,0313326 | 67,1767521 | 64,7896899 |

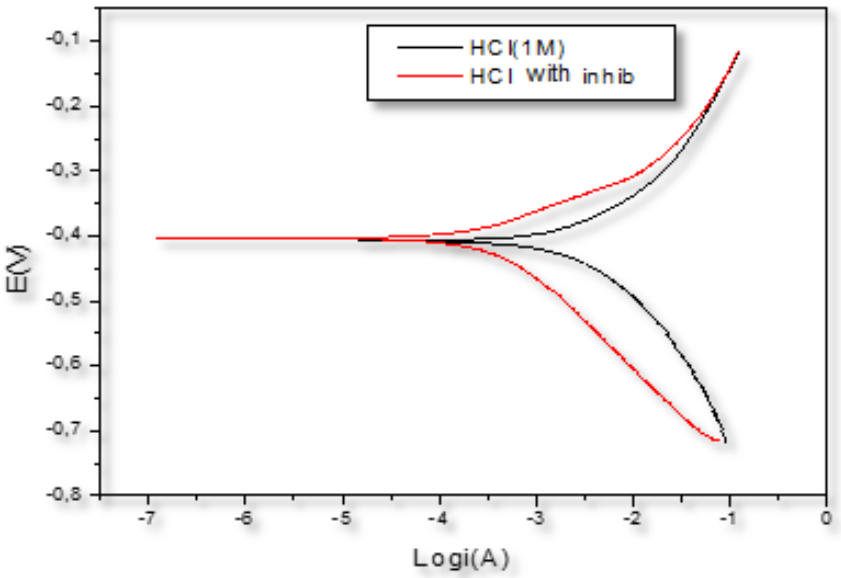


Fig 1 : Polarization curves of X70 steel in HCl medium (1M) without and with the inhibitor.

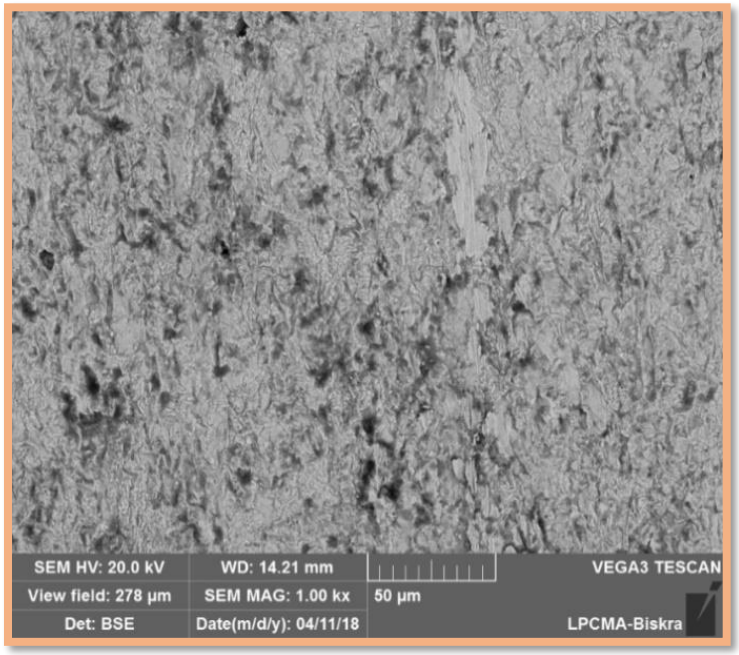


Fig 2 : Morphologic of surface on HCl (1M) + inhabit 14 day

# P11. Ultra-small iron oxide nanoparticles synthesized by gamma irradiation

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Superparamagnetic nanoparticles iron oxide ($Fe_3O_4$) were synthesized by radiolytic method in the presence of arabic gum (AG) as a biocompatible stabilizer in new biomedical applications. The gamma-irradiation method represents a powerful alternative way for the synthesis of monodisperse nanoparticles. In order to understand their mechanism formation under gamma irradiation, UV-Visible analyses of the absorbance have been carried out at different time during the irradiation process. Structural and magnetic properties are investigated using X-ray diffraction (DRX), transmission electronic microscopy (TEM), and SQUID magnetometer, respectively. The TEM observations and XRD analysis confirm the formation of the ultra-small magnetite nanoparticles (≈ 3.8 – 5.6 nm) in spinel structure. From magnetization measurements (Figure 1), it is shown that for radiation-induced particles are superparamagnetic at room temperature with higher average magnetic moments of $\mu_B$ = 2039 (100 K) and $\mu_B$ = 5547 (300 K) per nanoparticle.

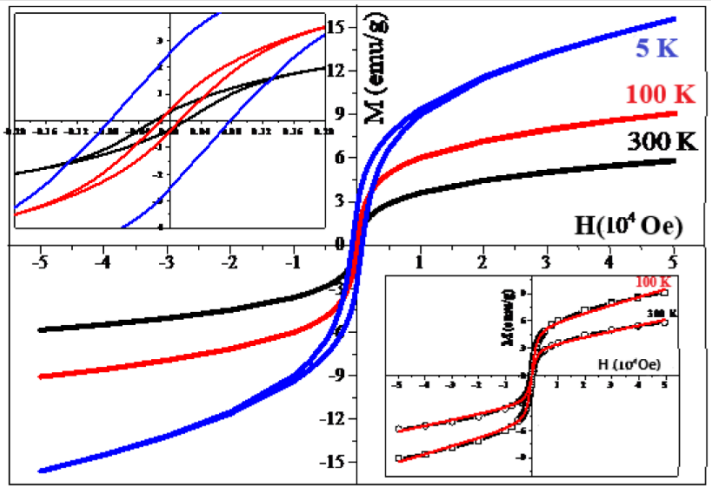


**Figure 1**: Magnetization hysteresis loops of radiation-induced $Fe_3O_4$ nanoparticles at $T$ = 5, 100 and 300 K. Insets: Left) Magnification of the low field region; Right) Modified Langevin in red function fit.

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# P12. Mechanical spectroscopy of $SiO_2$/Si, nanocomposites of multiwalled carbon nanotubes and polyamide, polyvinyl chloride, polyethylene, porous polystyrene

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After electron irradiation in figure 1 as a result of the collision of electrons $e^-$ with Si atoms Frenkel defects: vacancy - interstitial atoms V-$Si_i$ are formed.

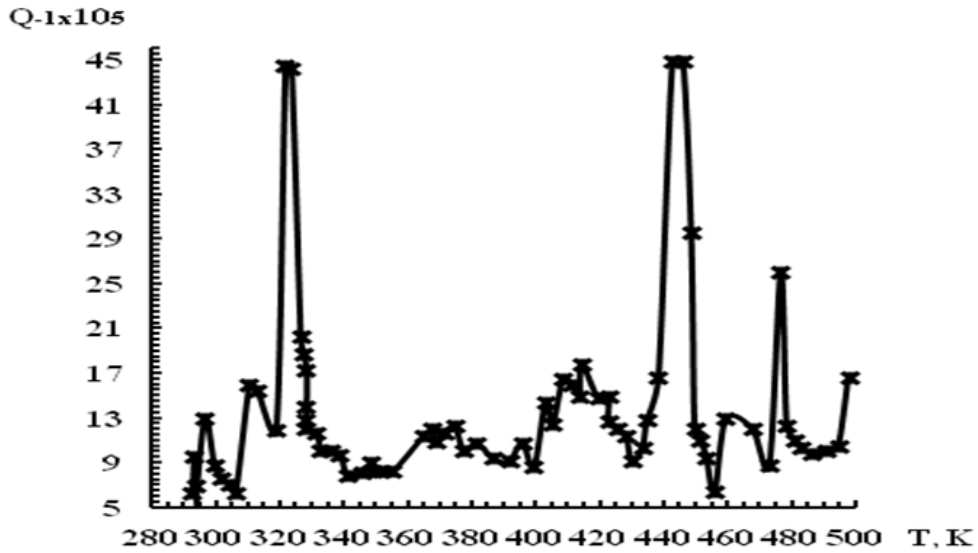


***Figure 1 -*** *Temperature dependence of internal friction $Q^{-1}(T)$ in $SiO_2$/Si wafer-plate p-type, doped with B, KDB-7.5(100) diameter $D \approx 76 \cdot 10^{-3}$ m, thickness $h_{Si} \approx 460 \cdot 10^3$ nm with $SiO_2$ layer thickness $h_{SiO2} \approx 100$ nm after electron with energy $W \approx 1,5$ MeV irradiation with energy $W \approx 1,5$ MeV dose $D_{e^-} \approx 10^{14}$ $cm^{-2}$*

## Conclusion

Internal friction $Q^{-1}$, elastic modulus E, shear modulus G, Poisson coefficient μ, depend on anisotropy of $SiO_2$/Si wafer-plate, of nanocomposites.

## Acknowledgements

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# P13. Optical and Morphological properties of $Nb_2O_5$ thin films grown by HiPIMS at room temperature

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Perovskite solar cells (PSCs) have shown remarkable progress in recent years with rapid increases in conversion efficiency, from reports of about 3% in 2006 to over 25% today [1]. Transparent and selective electrodes are crucial for PSCs performance. In particular, niobium pentoxide ($Nb_2O_5$) is a promising material to be used as electron selective layer due to its high stability [2]. Additionally, $Nb_2O_5$ is non-toxic and derives from readily inexpensive source materials. In this work, $Nb_2O_5$ thin films were grown on quartz slides at room temperature. A 1kHz High-power impulse magnetron sputtering (HiPIMS [3]) source at a power of -600 V on pulse and different duty-cycle was used. Optical reflection and transmittance were measured using a UV-Vis-NIR spectrometer (Lambda 750, Perkin Elmer) over the wavelengths from 190 nm to 2500 nm. All samples show average transmittances greater than 80% in the visible region. The refractive index of $Nb_2O_5$ thin films is around 2.4. Surface morphology was measured with atomic force microscopy (XE-100, Park Instruments) operating in air. All AFM images of the films were analyzed using scaling concepts. The wettability behavior was measured using a Goniometer (DSA25E, Kruss). $Nb_2O_5$ surface shows a contact angle lower than 50º.

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# P14. Development of magnetic PLA/CaP composites

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Polylactic acid (PLA) is a thermoplastic polyester that has been highly explored in tissue engineering applications due to its combination of mechanical properties and biocompatibility [1]. However, limitations related to bioactivity and biodegradability demand the development of PLA-based composites [2]. The addition of calcium phosphate-based (CaP) bioceramics as hydroxyapatite (HA) and/or β-tricalcium phosphate (β-TCP) to PLA-base matrix could be a solution to enhance mechanical and thermal properties, as well as degradability. The high attention of these composites is evidenced by their interest as feedstock for additive manufacturing technologies as fused filament fabrication [3]. Additionally, several studies have demonstrated that enhanced magnetic susceptibility, which is commonly accomplished by the use of magnetic nanoparticles (MNP), increase considerably these composites´ biological performance [4].

The main purpose of this research was the development of magnetic injection moulded PLA-based biocomposites by incorporating intrinsically magnetic iron-doped biphasic calcium phosphate particles (FeBCP) into the polymeric matrix by melt compounding. In contrast to the sole incorporation of MNP, whose long-term side effects are still unclear, this strategy aims to improve the magnetic susceptibility of the composite by using iron ions as dopants in CaP-based powders. The chemical, thermal, mechanical, and magnetic properties of the resulting biocomposites were compared to similar non-doped BCP biocomposites containing different amounts of BCP, as well as neat PLA. FeBCP/PLA composites presented a homogeneous distribution of CaP-based particles within the polymeric matrix, exhibiting a typical ferromagnetic-like behavior. Higher tensile strength than PLA or even non-doped composites, was also noticeable for magnetic biocomposite. The results presented in this work show the feasibility of developing a new generation of magnetic PLA-based composites without MNP incorporation, providing an opportunity for future and potential developments of new materials for hard tissue regeneration.

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# P15. Novel thermoelectric composites based on n-type $SrTiO_3$ for high-temperature energy harvesting

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Energy is the primary form of human activity and can be expressed in many forms, such as chemical, thermal, acoustic, electrical and many others. The most important is electricity, being the most used by the consumers, and there are many forms to produce it. Fossil fuels are still used for this purpose, but green solutions are preferable to avoid the environmental impacts. During electricity production, a significant part of the energy is lost as thermal energy. The energy efficiency can be improved by employing thermoelectric devices, which allow converting of the heat flux back to the electrical energy. A significant challenge is represented by thermoelectric conversion at high temperatures, requiring stable and performing materials. From those, oxides, and $SrTiO_3$-based compounds in particular, are especially promising for the high-temperature thermoelectric conversion.

This work is focused on the development of composite thermoelectric materials based on strontium titanate. The novel material design approach is based on A-site deficient donor-substituted $Sr_{0.85}La_{0.10}TiO_3$ matrix composition containing $SrMoO_3$ addition. Sintering such composites under reducing conditions results in specific microstructures, where the matrix grains are modified by the inclusion of $SrMoO_3$ fragments, with simultaneous formation of metallic Mo nanoparticles. The results demonstrated various combined effects in such structures, resulting in significant enhancement of the thermoelectric performance (achieving a power factor around 829 $mW/mK^2$, at 1165 K, to a sample of 98% molar of $Sr_{0.85}La_{0.10}TiO_3$ and 2% molar of $SrMoO_3$). Guidelines for such behaviour are discussed. Fabrication of the unileg thermoelectric modules and corresponding testing under relevant atmospheres was also attempted. The preliminary results show that such materials can be used for thermoelectric harvesting under oxidizing conditions.

# P16. Agarose hydrogels modified by silk fibroin as materials with tunable transport and rheological properties

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Extracellular matrix (ECM), the basis for living cells, has the character of hydrocolloid, but it mainly consists of two parts – fibrous (elastin, collagen) and amorphous (PG's, GAG's). It is a structurally very complex material however it can be simplified as a hydrogel matrix with fibers inside. Agarose is linear polysaccharide derived from seaweed which is a biocompatible material that forms hydrogel. Silk fibroin is a protein derived from silkworm cocoons. Both agarose and fibroin are widely used in medical and tissue engineering applications. In this study simple hydrogels were formed, that consist of fibrous component (silk fibroin), in an amorphous component (agarose hydrogel) and the effect of addition silk fibroin on transport and rheology properties was studied. Silk fibroin was extracted from raw silk fibers using Ajisawa's reagent [1]. Samples were prepared with two different concentrations of agarose (0,5 and 1,5 wt. %) and two different concentrations of silk fibroin (2,0 and 5,0 wt. %). Rheology properties were studied by amplitude and frequency sweep tests (Anton Paar MCR 72) and effective diffusion coefficients were determined by the diffusion model of the constant source (concentration of methylene blue in dependence on the distance from the hydrogel/solution interface was determined using UV-VIS spectrometry - Cary50, Varian). In all samples the diffusion of methylene blue was slower than in water. For the samples which contained only agarose, the diffusion was slower with increasing agarose concentration. The diffusion for the samples with fibroin was decreasing with increasing fibroin concentration. Viscoelastic modules were decreasing with decreasing agarose concentrations and decrease with the fibroin presence. High concentrated fibroin enhances the mechanical properties of low concentrated agarose, on the other hand, fibroin weakens mechanical properties of high concentrated agarose. Hydrogels with tunable transport and mechanical properties can be tailored by using specific ratio of fibroin and agarose. Using different concentrations of these materials can provide desired materials for specific applications.

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# P17. Synthesis of Zeolite H-ZSM-5 for Fischer Tropsch synthesis

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Nowadays, petroleum is one of the main sources of production of fuels as well as of a large number of chemicals. The Fischer-Tropsch synthesis appears as one of the main alternative methods. [1]. In this study, we aim to investigate whether encapsulating a Co/ZSM-5 and Co/H-ZSM5 Fischer-Tropsch synthesis catalyst in hollow carbon spheres will improve its selectivity to $C_{5+}$ hydrocarbon chains.

ZSM-5 have been synthesized using steam-assisted crystallization method at two different Si/Al ratios and we obtained respectively two zeolites designated as ZSM-$5_1$ and ZSM-$5_2$. Tetrapropylammonium hydroxide (TPABr) as the soft organic templating agent has been used. Ion exchange was further performed using a 1M solution of $NH_4NO_3$ at 80˚C for 4h to obtain H-ZSM-$5_1$ and H-ZSM-$5_2$. Co/H-ZSM-5 preparation was achieved by impregnation. The next step is the encapsulation of Co/H-ZSM-5 by hallow carbon sphere to obtain (Co/H-ZSM-5@HCS). The purpose of this encapsulation is to have a very good catalyst which can improve the products of Fischer-Tropsch analysis. Thus we can help developing countries in the production of fuel with this method. Any preparation of mesoporous zeolite first requires a source of pure silica and a source of aluminum and after their preparation, we need to characterize them in order to know a certain number of parameters to be sure that the zeolite is suitable for the purpose of obtaining selective Fischer-Tropsch products [2]. Various techniques were used to characterize the catalysts *viz* BET, XRD, SEM, FTIR, and TGA.

According to these results, we can say that we have successfully obtained our Co/H-ZSM-5 and we will see how to encapsulate carbon on it to have Co/H-ZSM-5@HCS for next step.

Some results were presented (figure.1: XRD, figure.2: FTIR, figure.3: TGA)

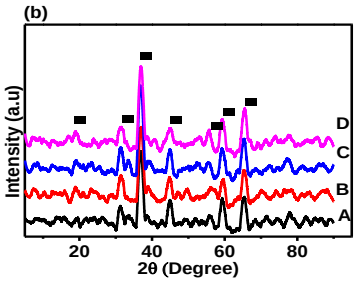


Fig. 1 : XRD

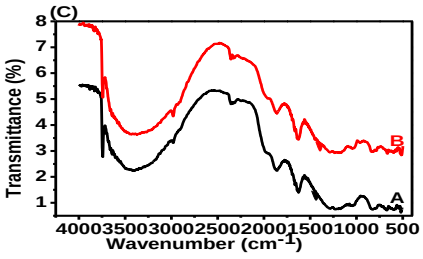


Fig.2 : FTIR

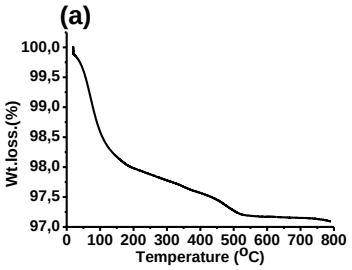


Fig.3 : TGA

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# P18. Cytocompatible gelatin/boronsilicate hybrid materials

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New hybrid materials capable to produce biodegradable scaffolds or films, targeted to tissue regeneration have gained increasing attention [1]. Among the various hybrid systems, the gelatin-silica system has presented interesting results, namely as a stand-alone material for scaffolds [2,3]. Gelatin-Borosilicate xerogels were developed in a way to include, in the inorganic domains of the hybrid system, ions recognized for enhancing bioactivity, such as calcium, strontium and boron [4]. The chemical structures of the hybrid material were analysed by FTIR, 1H MAS (magical angle spinning), 29Si MAS, 29Si-{1H} CP-MAS (cross-polarization magical angle spinning) and 11B HAHN-ECHO NMR. Mouse fibroblast cell line L929 was used for cytotoxicity evaluation, showing a good response to the materials after seven days.

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# P19. Advantages of using sequential chemical fractionation to alkaline extraction for accessing the organic matter in biochar.

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This contribution is focused on utilization of a sequential chemical fractionation method for determination of organic matter content, its distribution in biochar and the possible use of biochar as a soil conditioner in agriculture. For these purposes the optimized chemical fractionation procedure [1,2] was used to reveal the content of organic matter in different biochar samples with different properties (samples with European biochar certification for usage in agriculture) which depend significantly on the temperature used during a pyrolysis of biomass residues in the process of biochar production. For the purpose of this study, a biochar from the Czech company BIOUHEL.cz was used. In parallel, these samples were also fractionated by classic alkaline extraction to obtain the so-called extractable fraction of organic matter (NOM – natural organic matter). Biochar is one of the important soil conditioners, known for having positive effect on crop yield, soil quality, nutrient cycle and carbon sequestration due to the transfer of organic carbon from it to the soil. However, the effect depends on the properties of the biochar, its doses to the soil, but also on the properties of the soil itself. Using the sequential chemical fractionation allowed us to separate all the different-strongly bound fractions of similar types of molecules. The alkaline extraction only allowed us to see a mixture of organic molecules contained but overall, this method wasn`t really good to use in order to separate the organic matter from biochar. Individual fractions obtained from sequential chemical fractionation as well as NOM samples were characterized by methods of elemental analysis (determination of organic elements content), thermogravimetry (contents of ash, organic matter and moisture). The results showed that the method of sequential chemical fractionation gives higher yields of organic matter compared to classical alkaline extraction. Overall, the analyzes show that the investigated biochar is a really rigid and durable material that, even after using of aggressive reagents and high temperatures, still contains a high amount of organic matter. The structure couldn`t be cleaved at a level where really strongly bound organic matter could be extracted, which is indicating the high resistance of organic matter in biochar structure. To be able to make more detailed description we will perform chromatographic analysis (GC-MS and LC-MS) which will provide us information on the molecular level of fractions or structural analysis methods (e.g. FTIR, NMR). Another follow-up research will include using these separation methods to characterize a biochar that has been cultivated and treated with soil microorganisms. That will make it possible to better assess their potential effect on biochar in the soil.

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# P20. Hydrogenated amorphous carbon-based coatings for orthodontics: bacterial adhesion

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Corrosion of orthodontic appliances inevitably occurs in vivo. In fact, the mouth is an ultimate corrosion-promoting environment, with oscillations in temperature, pH and chemical composition, and hosting over 700 known bacterial species that can form biofilms on any surface. Different types of corrosion were identified, including pitting, fretting and microbiologically induced corrosion (MIC), which consequently release metallic ions into the oral cavity. Among the released ions, Ni stands as local to systemic symptoms of Ni allergic reactions to metallic orthodontic components are described in the literature. Moreover, Ni ions can trigger cytotoxic and mutagenic effects, induce DNA damage and apoptosis, and modify gene expression. Therefore, protecting widely used orthodontic alloys – such as stainless steel (SS) and NiTi – is of utmost importance. A solution from Surface Engineering is coating the surface to protect the substrates from corrosion. Among the available materials, hydrogenated amorphous carbon (a-C:H) is a potential candidate not only for its mechanical and tribological properties but also for its outstanding biocompatibility and bioinertness.

In this research work, hydrogenated amorphous carbon (a-C:H)-based coatings, included in the Diamond-Like Carbon (DLC) materials, were deposited on the medical grade SS 316L AISI by reactive magnetron sputtering. Previous research work [2–4] suggested that a-C:H-based coatings are both biocompatible and offer protection against *in vitro* corrosion in artificial saliva. This study evaluates the *in vitro* bacterial adhesion of *Staphylococcus aureus* UCCCB115, *Bacillus subtilis* UCCCB117 and *Pseudomonas aeruginosa* UCCCB116 on a-C:H-based coatings for orthodontic applications. The ability to colonize the surface of the material was evaluated by SEM/EDS and colony-forming units enumeration, after a 24-hour incubation at 37ºC. Raman, FTIR, AFM and SEM/EDS performed the microstructural characterization of the coatings.

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# P21. Synthesis, Characterization of Three Distinct Phases of Bismuth Molybdate for Supercapacitor Applications

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The three distinct phases of Bismuth Molybdate is employed for supercapacitor applications. Bismuth Molybdates are synthesised via the sol-gel method and characterization studies were carried out for the size, crystallinity, and morphology of the as-synthesised molybdates. XRD confirm the monoclinic structures of α-$Bi_2Mo_3O_{12}$ and β- $Bi_2Mo_2O_9$ and the orthorhombic structure of γ- $Bi_2MoO_6$. Raman spectroscopies verify the phase purity of the as-synthesised samples. The optical properties and the bandgap is investigated using UV Absorbance and Reflectance spectroscopy. Electrochemical studies such as Cyclic Voltammetry (CV), Galvanostatic Charge Discharge (GCD), and Electrochemical Impedance Spectroscopy (EIS) were carried out. Thus the fascinating electrochemical behaviour of Bismuth Molybdates suggests their utilization in energy storage systems.

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# P22. Synthesis and Characterization of pure β-$Bi_2Mo_2O_9$ and Eu-doped β-$Bi_2Mo_2O_9$ for Photocatalytic applications

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One of the phases of Bismuth Molybdate is studied for photocatalytic activity. The pure β-$Bi_2Mo_2O_9$ and Eu doped β-$Bi_2Mo_2O_9$ synthesised using the sol-gel technique is observed in both water and acetic medium. The XRD and Raman studies confirm the monoclinic structure of β-$Bi_2Mo_2O_9$. The surface morphology of synthesised nanoparticles shows the formation of a honeycomb-like shape with numerous porous structures. The photocatalytic activity was demonstrated by the dye degradation process under visible light radiation. The dye taken into account for photocatalytic activity is Methylene Blue. The absorbance of the synthesised β-$Bi_2Mo_2O_9$ $i_n$ acetic and water medium and Eu doped β-$Bi_2Mo_2O_9$ with varied concentrations were studied by UV-Visible spectrophotometer. The results demonstrate that water-based β- $Bi_2Mo_2O_9$ degrades more dye than acetic-based β - $Bi_2Mo_2O_9$. However, doping Eu into pure β - $Bi_2Mo_2O_9$ results in a significant boost in photocatalytic degradation efficiency over water-based pure β - $Bi_2Mo_2O_9$. Within 4 hours, the 10% Eu: $Bi_2Mo_2O_9$ destroyed the Methylene Blue dye (100%).

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# P23. Development of 2D $MoS_2$ nanosheets on Lotus fibres for enhanced Hydrophobicity and Anti-microbial activity

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The cellulose threads obtained from Lotus (Nelumbo nucifera) are studied for their enhanced hydrophobicity and anti-microbial activity upon coating with 2D $MoS_2$ nanosheets. The $MoS_2$ synthesised by the co-precipitation method is coated on the obtained lotus fibres. XRD and SEM studies confirm the crystallinity and morphology of the as-synthesised $MoS_2$. SEM confirms the formation and deposition of $MoS_2$ on the pure cellulose fibres. Anti-microbial studies were carried out using *Escherichia Coli* and *Candida albicans.* Anti-microbial studies further validate that the threads@$MoS_2$ results in better activity than the uncoated fibre. Because of their increased hydrophobicity, $MoS_2$ sheets play a significant role in limiting the wicking potential of pure threads and thus threads@$MoS_2$ shows no penetration which might be incorporated into textiles as well.

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# P24. Room temperature synthesis and characterization of ZIF-8

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Metal Organic Frameworks (MOFs) whose structure is composed of metal ions and organic ligands are novel porous materials [1]. Because these materials have numerous synthesis methods and types, it can be possible to use MOFs in a wide range of applications such as carbon dioxide capturing [2], hydrogen storage [3], gas separation [4], heterogenous catalysis [5]. As a subclass of MOFs Zeolitic Imidazolate Frameworks (ZIFs) are formed by assembling N atoms which originate from Imidazolate ligand and transition metals (Zn or Co). ZIF-8 which was produced nearly 15 years ago firstly is the most eminent member of ZIFs because of its thermal and chemical stability, porosity and huge surface area [1]. The aim of the study was to synthesize ZIF-8 at room temperature by utilizing solvent. We used methanol (MeOH) which was classified as relatively environmental friendly solvent [6]. Molar ratio in synthesis mixture was adjusted as $Zn^{2+}$: 7.9Hmim (2-methyl imidazole): 695 MeOH [7]. X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR) techniques were used to determine the properties of synthesized nanomaterial.

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# P25. Plastic waste as optimum feedstock for CD-based anticounterfeit tracers

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The fabrication of luminescent carbon dots (CDs) which allow the design of unique optical fingerprints in a polymer matrix, is a novel and exciting technology for tracing and security control of polymeric products. CDs are considered a new emerging class of 0D carbon-based luminescent nanomaterials with a size bellow 10 nm and a quasi-spherical morphology, composed of $sp^2/sp^3$ carbon-core. They hold many advantages like low cost, broad excitation spectra, tunable emission spectra and stable photoluminescence. These carbon nanoparticles can be obtained, in theory, from any carbon-based material. The focus of this work is the study of the upcycling of plastic waste, with the objective of obtaining a valuable product from common use plastic waste. Therefore, a reactor was built up for the large-scale production of CDs using most common types of polymers, namely polylactic acid (PLA).

The experimental procedure is known as Flash Joule Heating (FJH), since the material is heated to a temperature exceeding 3000K in milliseconds, due to the electrical current. The polymeric material is converted to a very high-quality graphene, which in turn would give rise to the desired CDs. [1] There are endless possibilities, but the aim is to explore the produced CDs as a fingerprint for the traceability and security of any polymeric-based product that can arrive to the end consumer, contributing also to the ever-growing problem of waste management.

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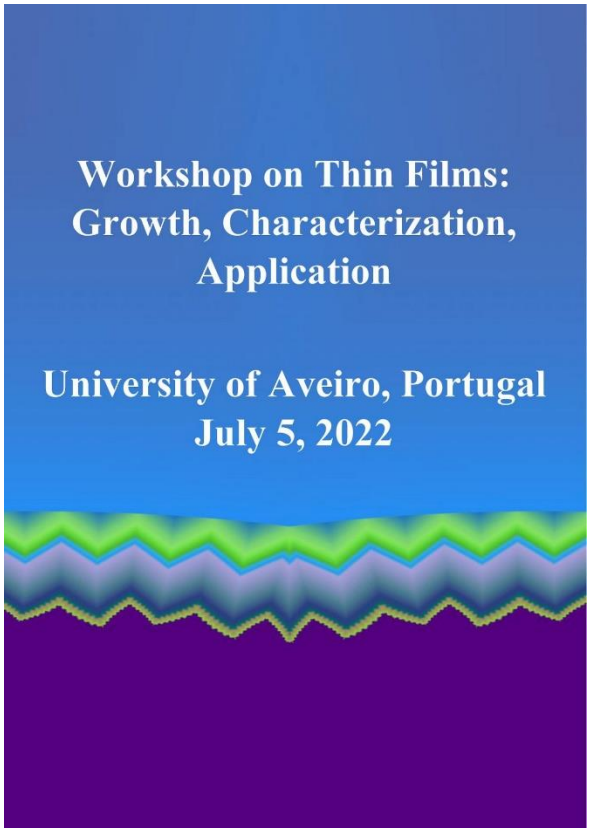
# Workshop 1

# Workshop on Thin Films: Growth, Characterization, Application

## University of Aveiro, Portugal
## July 5, 2022




Thin films as a special type of matter have been in the focus of theoretical and experimental research for many years. Advances in thin film have enabled a wide range of technological breakthroughs in all areas of our live: energy, electronics, constructions, medicine, communications, transport, etc. Many fundamental and technological questions related to thin films have not yet been resolved. Workshop on Thin Films: Growth, Characterization, Application (WTF2022) will be devoted to reviews and discussions of the most important, modern, relevant areas of physics, chemistry, and technology of thin films.

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| **Workshop on Thin Films: Growth, Characterization, Application**<br>**University of Aveiro, Portugal July 5, 2022 (*online*)**<br><br>**Auditorium 1.** | |
| **9:00-9:15** | **WELCOME ADDRESS**<br>**Prof. Dr. Duncan Paul Fagg, Dr. Igor Bdikin** |
| **9:15-10:15** | CHAIR: Prof. Dr. Duncan Paul Fagg<br><br>***Plenary Lecture***<br><br>**Deposition of complex oxide thin films by multitarget reactive sputtering**<br>**Prof. Dr. Gunnar Suchaneck**<br>*Solid State Electronics Laboratory, Dresden University of Technology, Germany* |
| **10:15–11:15** | CHAIR: Prof. Dr. Duncan Paul Fagg<br><br>***Plenary Lecture***<br><br>**Deposition of diamond films by chemical vapor deposition**<br>**Dr. Joana Catarina Mendes**<br>*Instituto de Telecomunicações AVEIRO, PORTUGAL* |
| **11:15–11:30** | **Final discussions and comments / Coffee break** |

# Multi-target reactive sputter deposition of complex oxide thin films

**Gunnar Suchaneck***

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Currently, thin film research is moving towards the fabrication of novel nano- and heterostructures consisting of thin film materials with three and more different cations, thereby often possessing complex microstructures.

The majority of reports dealing with sputter deposition complex oxide thin films has been conducted through RF magnetron sputtering (MSP) of a high-temperature sintered ceramic targets. Multi-target reactive sputtering (MTRS) of perovskite oxides was introduced in 1980ies for the fabrication of $Pb(Zr,Ti)O_3$ (PZT) thin films.

After a general introduction in peovskite thin film deposition, the first part of this talk is devoted to MTRS first of in-situ crystallized PZT thin film deposition on silicon wafer comprising an insulating $ZrO_2$ buffer layer or a Pt(111) bottom electrode. In order to meet the criteria for a cost-effective industrial deposition process, the deposition was done on four 6″ diameter silicon wafers per run. Three metallic (Pb, Ti, Zr) targets with high purity, each of 8″ diameter, were reactively sputtered. A thin $TiO_2$ seed layer, which in the ideal case disappears in further deposition, was used as a seed layer and to avoid a lead-deficient interface. Film composition was controlled in-situ by means of a plasma-emission monitor. MTRS allowed the fabrication of self-polarized PZT thin films for pyroelectric and piezoelectric applications. Advanced characterization techniques – multi angle spectroscopic ellipsometry, laser intensity modulation method, piezoelectric force and Kelvin probe force microscopy – were applied to obtain profiles of optic, pyroelectric, piezoelectric properties as well as of the surface potential. Second we demonstrate film deposition of of a more complex perovskite material - PMN-PT. Third, we consider the deposition of lead-free $Ba(Zr,Ti)O_3$ for application in electrocaloric cooling devices. Microstructure, texture, phase composition, optical and piezoelectric properties are considered. A device demonstrator is presented. Finally, some results of $Sr_2FeMoO_{6-\delta}$ thin film deposition for spintronic devices are reported.

Workshop on Thin Films: Growth, Characterization, Application

# Deposition of diamond films by chemical vapor deposition

**Joana Catarina Mendes**

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The extreme properties of diamond make it a material with tremendous potential for engineering applications. Its high Young modulus, wear resistance and chemical inertness open the door for tribological applications. On the other hand, diamond's high bandgap, breakdown electric field and thermal conductivity make it an interesting material for high power and high temperature electronic applications. In the field of electrochemistry, it is extremely resistant to oxidation and attack by acids, even at high temperatures; these properties, together with the possibility of doping, allow the fabrication of diamond electrodes and sensors. However, these applications rely on the possibility of depositing diamond films on different types of substrates. This can be done by chemical vapor deposition (CVD). With this technique, diamond films have been deposited on a variety of materials, like diamond single crystals, tools and electronic materials. This paper will describe how diamond films can be grown by CVD on different substrates, the challenges of the process, and the different types of CVD systems. It will also review the main areas of application of CVD diamond.

# Workshop 2

# Workshop on Modern Problems of Workshop on Modern Problems of Bionanomaterials: Science, Technology, Application

University of Aveiro, Portugal July 5, 2022


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 our days developing of biomaterials, nano science and information technology give optimistic perspectives on this way. But this allows see 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 solve new questions in these areas. For help in this we organize Workshop on Modern Problems of Bionanomaterials: Science, Technology, Application (WMPB2022) with presentations and discussions specialists in Biomaterials, Nano science and Nano technology.

**Workshop on Modern Problems of Bionanomaterials: Science, Technology, Application**
**University of Aveiro, Portugal July 5, 2022**

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**Workshop on Modern Problems of Bionanomaterials: Science, Technology, Application**
**University of Aveiro, Portugal July 5, 2022**

**Auditorium 1.**

CHAIR: Dr. Gil Gonçalves

| | |
|---|---|
| **11:30–12:15** | **W2-O1. Problems of atomic force microscopy of organic materials**<br>**Dr. Igor Bdikin**<br>*TEMA, Department of Mechanical Engineering, University of Aveiro, Portugal* |
| **12:15–14:00** | **Lunch break** |
| **14:00–15:00** | ***Plenary Lecture***<br>**Review Lecture on Workshop on Modern Problems of Bionanomaterials: Science, Technology, Application**<br>**Prof. Dr. José M.F. Ferreira**<br>*Department of Materials and Ceramic Engineering (DEMaC), University of Aveiro, Portugal* |

# Review Lecture on Workshop on Modern Problems of Bionanomaterials: Science, Technology, Application

**José M. F. Ferreira**

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Synthetic bone grafts are commonly based on calcium phosphates and bioactive glasses (BGs). Biphasic calcium phosphate ceramics (BCPs) comprising a mixture of hydroxyapatite (HA) and β-tricalcium phosphate (β-TCP) are considered better in comparison to either single-phase HA or β-TCP components. Even though, BCPs do not accurately mimic the inorganic part of the bone, which also contains trace amounts that play essential therapeutic roles on bone metabolism. Bioactive glasses (BGs) elicit special responses when in contact with biological fluids in a way that depends on the composition. Therefore, fine tuning the chemical composition of these materials is the way to engineer bone grafts with enhanced performance *in vitro* and *in vivo*.

Bone grafts can be engineered in a variety of forms (thin films, membranes, granular bone fillers, injectable formulations, porous scaffolds, etc.). This presentation will provide an updated overview about the ongoing research activities in the specific area of synthetic bone grafts. Special emphasis will be given to the compositions of starting materials and to the easiness of processing (scaffold fabrication by additive manufacturing and sintering). An alternative approach is taking advantages of natural marine-derived porous structures to engineer multifunctional devices.

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Workshop on Modern Problems of Bionanomaterials:
Science, Technology, Application

# W2-O1. Problems of atomic force microscopy of organic materials

**Igor Bdikin**

*TEMA, Department of Mechanical Engineering, University of Aveiro, Portugal*

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

For effective commercial devise there several parameters: technological problems and cost, bio and ecology acceptability, value used for the practical application of the effect. Here we show the applicability and current problems of piezoresponse force microscopy (PFM) for studying a broad range of polar materials at the nanoscale for biological / organic complex materials: organic polymers [1], organic nano tubes [2], amino acids/ nucleobase [3], organic fibers [4], organic composite films [5], organic single crystals [6].

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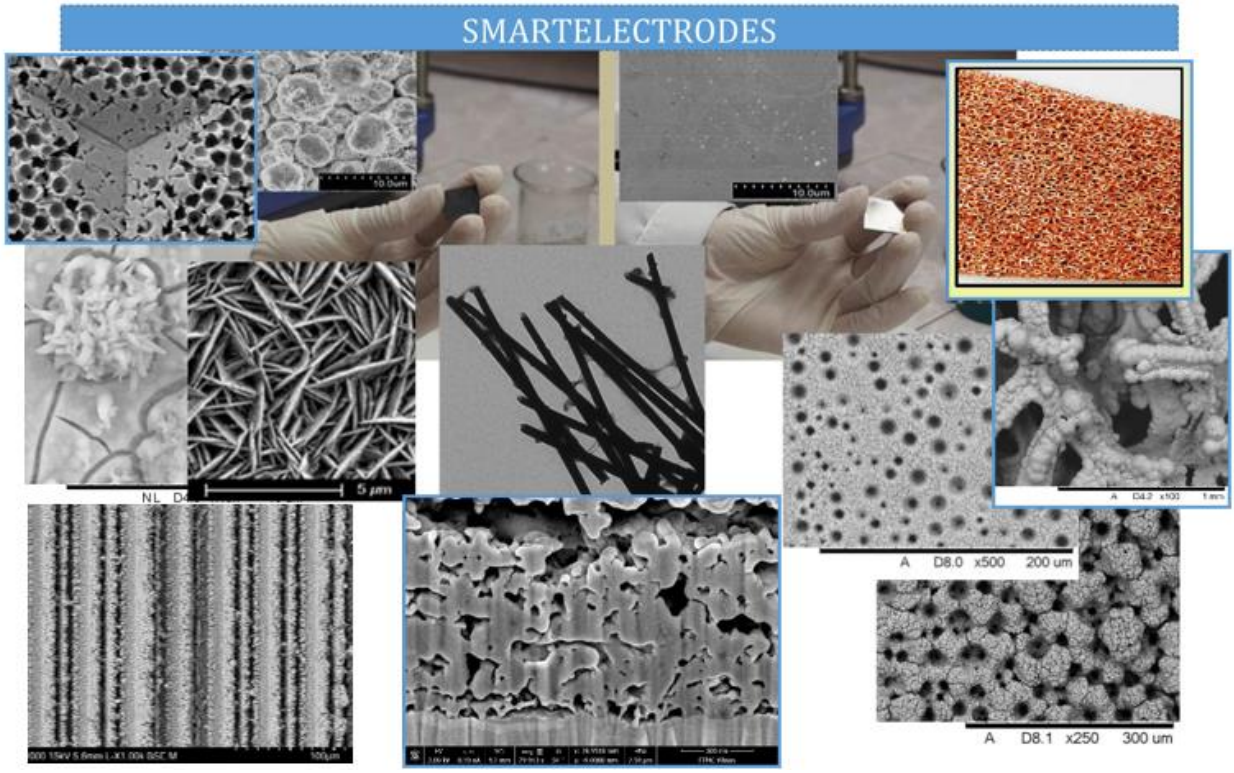
# Workshop 3

# "SMARTELECTRODES" Workshop: **Smart metallic and semiconductor materials: synthesis, characterization, applications and challenges.**

Demand of "smart" electrodes/systems has recently increased due to significant role of various devices/equipment based on these materials; e.g. electrochemical/electrophysical applications as catalysis/electrocatalysis, sensoring, thermoelectrics, electrowinning, electrochemical machining and electrospark alloying. The development of multiscaled (from nano- to macro-; from nanowires to volumized 3D-) metallic and semiconductor electrodes and integration of them into working systems/equipment is the main target of S**MARTELECTRODES**




Online workshop organized in the framework of 5th International Conference on Nanomaterials Science and Mechanical Engineering, **ICNMSME-2022**, University of Aveiro, Portugal, 2022.

Lectures are presented by participants of **SMARTELECTRODES** project (Grant agreement: 778357), Marie Skłodowska-Curie Research and Innovation Staff Exchange program.

More information about the project is available at: https://www.smartelectrodes.eu/

**Topics**: films/coatings, metallic foams, electrowinning, semiconductor, nanostuctured materials; catalytic, thermoelectric, sensing applications, electrochemical impedance spectroscopy

**"SMARTELECTRODES" Workshop: Smart metallic & semiconductor materials: synthesis, characterization, applications and challenges**
**University of Aveiro, Portugal,**
**July 5, 2022**

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**"SMARTELECTRODES" Workshop: Smart metallic & semiconductor materials: synthesis, characterization, applications and challenges**
**University of Aveiro, Portugal,**
**July 5, 2022**

**Auditorium 2.**

*Keynote presentations*

**Chairs: Prof. Henrikas Cesiulis, Dr. Natalia Tsyntsaru**

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|---|---|
| **11:30 – 11:55** | **W3-O1.**<br>***Development of technological electrodes/processes at EPT and TOPAZ companies within SMARTELECTRODES project***<br>**Dr. Natalia Tsyntsaru**,<br>*Vilnius University, Lithuania/ Institute of Applied Physics, Moldova* |
| **11:55 – 12:20** | **W3-O2.**<br>***Application of electrochemical impedance spectroscopy (EIS) for processes and systems characterization***<br>**Prof. Dr. Henrikas Cesiulis**<br>*Vilnius University / EPT , Lithuania* |
| **12:20 – 12:45** | **W3-O5.**<br>***$Mo_xS_y$-containing coatings for photo/electrochemical water splitting applications***<br>**Dr. Ramunas Levinas**<br>*Vilnius University, /FTMC , Vilnius, Lithuania* |
| **12:45 – 14:00** | **Lunch break** |
| **14:00 – 14:25** | **Chairs: Prof. Henrikas Cesiulis, Dr. Natalia Tsyntsaru**<br>**W3-O6.**<br>***Nanomultilayer structures based on chalcogenide amorphous semiconductors: obtaining and applications***<br>**Dr. Alexei Mesalchin**<br>*Institute of Applied Physics, Chisinau, Moldova* |
| **14:25 – 14:50** | **W3-O4.**<br>***Functional properties of Fe-Ga alloys prepared by electrodeposition***<br>**Dr. Aliona Nicolenco**<br>*Marie Curie fellow, Universitat Autònoma de Barcelona, Spain/ Institute of Applied Physics, Moldova* |

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|---|---|
| **14:50 – 15:15** | **W3-O7.**<br>***Electrodeposited Co-Mo Composites with Titania for the Hydrogen Evolution Reaction***<br>**Dr. Cheng Wang**<br>*Microfabrica Inc, CA / Clarkson University, USA* |
| **15:15 – 15:40** | **W3-O3.**<br>***Electrodeposited Alloys for the Oxygen Evolution Reaction (OER)***<br>**Prof. Dr. Elizabeth Podlaha-Murphy**<br>*Clarkson University, USA* |
| **15:40 – 15:50** | **Final discussions and comments** |

"SMARTELECTRODES" Workshop: Smart metallic and semiconductor materials: synthesis, characterization, applications and challenges

# W3-O1. Development of technological electrodes/processes at EPT and TOPAZ companies within SMARTELECTRODES project

**N. Tsyntsaru** [1,2,*], H. Cesiulis[1,3], I. Bulan[4]

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H2020-MSCA-RISE SMARTELETRODES project is devoted to multiscaled smart metallic and semiconductor electrodes for electrochemical / electrophysical processing and devices. Demand of "smart" electrodes/systems has recently increased due to significant role of various devices/equipment based on these electrodes used for versatile applications. The smartelectrodes play significant roles in several areas such as catalysis/electrocatalysis, magnetic, sensoring, thermoelectrics, electrowinning, electro-spark alloying (ESA), electrochemical machining.

3D-electrodes (industrial copper foam) for electrocatalysis and electrowinning, i.e. for applications demanded an enhanced area of working surface were investigated at premicies of JSC "EPT". These electrodes are promising because of their high rigidity, light weight (density <1 g/cm$^3$), flexibility of shapes. It was determined that mass transfer is ~3 times faster, and specific surface area is ~15 times higher compared to the plane surface. These electrodes were used for electrowining of Cu, Sn, Pb from solutions obtained in the process of metals recovery from e-waste.

The pulse synthesizer developed at JSC "TOPAZ" allowed to control energy of the ESA process more accurately. Such precise doping technology is especially important while working with "problematic" substrates (such as titanium, nickel), or vice versa applying very expensive palladium-iridium layers. Electro-spark alloying performed at TOPAZ installations could increase significantly (2 ÷ 10 times) such service characteristics of parts and tools as wear resistance, fretting resistance, heat resistance, antifriction properties.

*Acknowledgements:* this work has received funding from the European Union's Horizon2020 research and innovation programme under the MSCA grant №778357-SMARTELECTRODES.

"SMARTELECTRODES" Workshop: Smart metallic and semiconductor materials: synthesis, characterization, applications and challenges.

# W3-O2. Application of electrochemical impedance spectroscopy (EIS) for processes and systems characterization

**H. Cesiulis**[1,2,*], N. Tsyntsaru [1,3]

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Electrochemical impedance spectroscopy (EIS) is a recent and powerful tool for characterization of electrochemical systems. EIS is also called AC Impedance or just Impedance Spectroscopy. The usefulness of impedance spectroscopy lies in the ability to distinguish the dielectric and electric properties of individual contributions of components under investigation. Impedance spectroscopy is a non-destructive technique and so can provide time dependent quantitative and time-dependent information about the electrode processes and complex interfaces, extract some characteristics of materials including high resistance materials (e.g. paintings, oxide coatings). Because EIS only probes the electrode-solution interface, it can be used to characterize various kinetic properties of the reaction under investigation. For example, the double layer capacitance is proportional to the electrochemically active surface area of an electrode immersed in solution, and the charge transfer resistance shows how readily the electrochemical reaction occurs. The method is particularly useful for non-destructive analysis of electrocatalysts.

IMPS (Intensity Modulated Photocurrent Spectroscopy), on the other hand, also probes the solid state, and can provide information on important photoactive material parameters: rate of charge carrier – hole recombination, rate of charge transfer through the semiconductor-electrolyte interface, capacitance of the space charge layer, and more. Both techniques can be combined for suitable materials, and would offer a comprehensive characterization of the material. The practical applications of EIS are targeting for the following film types: (i) cathodic metals/alloys films deposition; (ii) mechanisms of metals and alloys corrosion; (iii) anodization of metals and characterization of oxide films and its growth by EIS including information provided by Mott-Schottky plots; (iv) underpotential deposition of metals; (iv) characterization of organic films onto metals; (v) application in development of biosensors and biofuel cells

*Acknowledgements:* this work has received funding from the European Union's Horizon2020 research and innovation programme under the MSCA grant №778357-SMARTELECTRODES.

"SMARTELECTRODES" Workshop: Smart metallic and semiconductor materials: synthesis, characterization, applications and challenges.

# W3-O3. Electrodeposited Alloys for the Oxygen Evolution Reaction (OER)

Yujia Zhang,[1] Ramunas Levinas,[2] Jūratė Petronienė,[2] Živilė Stankevičiūtė,[2] Arash Baharololoomi,[1] Natalia Tsyntsaru,[2,3] Henrikas Cesiulis[2] and **Elizabeth Podlaha-Murphy**[1,*]

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**Purpose**: Earth-abundant Fe-Ni-Co oxides are recognized as very good oxygen evolution reaction (OER) electrocatalysts for water splitting electrolysis [1]. Tungsten trioxide, $WO_3$, is a demonstrated photoanode although suffers from high recombination of photon generated electron–hole pairs, that can be mitigated by a $TiO_2$ heterojunction [2]. In the present work, conditions to electrodeposit Fe-Ni-Co alloy thin films and composites with $WO_3$-$TiO_2$ containing nanoscale $TiO_2$ particles, are identified in order to improve OER electrocatalysis. UV irradiation is used as a probe to understand the behavior of the composite.
**Materials and Methods**: Fe-Ni-Co alloy thin films were electrodeposited onto copper electrodes from a boric acid electrolyte containing nickel sulfamate, iron and cobalt sulfate. Deposition occurred over a range of current densities onto both rotating and stationary electrodes. The partial current densities were determined and the material composition and morphology characterized. OER electrocatalysis of the Fe-Ni-Co alloys and composites was examined.
**Results**: Electrodeposited Fe-Ni-Co alloys exhibited an anomalous codeposition behavior resulting in a range of iron-rich composition that catalyzed OER particularly at high current density. Incorporating the $TiO_2$ into a $WO_3$ matrix, without Fe-Ni-Co, significantly improved OER electrolysis but only exhibited a small photoelectrochemical increase in rate with UV irradiation. Combining Fe-Ni-Co/$WO_3$-$TiO_2$ lead to a synergistic improvement in OER under visible light. UV irradiation experiments and evidence from IMPS spectra, showed composite films containing both $WO_3$ and $TiO_2$ exhibited significant recombination kinetics.
**Conclusions**: Conditions were identified to electrodeposit an iron-rich alloy and composite with $WO_3$-$TiO_2$ that exhibited enhanced OER current density in visible light, but degraded in UV light.
**Acknowledgements**: this work has received funding from the European Union's Horizon2020 research and innovation programme under the MSCA grant №778357-SMARTELECTRODES.

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"SMARTELECTRODES" Workshop: Smart metallic and semiconductor materials: synthesis, characterization, applications and challenges.

# W3-O4. Functional properties of Fe-Ga alloys prepared by electrodeposition

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Fe-Ga alloys have a unique combination of mechanical and magnetic properties, as well as desirable magnetostriction, i.e., the ability to change dimensions in response to an applied magnetic field [1]. These functional properties enable the use of Fe-Ga alloys in various sensors and actuators operating under harsh mechanical conditions [2]. Nevertheless, traditional Fe-Ga fabrication methods rely on physical deposition techniques that limit the opportunities for materials design at the nanoscale. In this work, Fe-Ga alloys with variable Ga content (up to 40 at.%) were prepared by electrodeposition, and the functional properties, i.e., mechanical, magnetic and magnetostrictive properties, were assessed as a function of alloys composition. Additionally, different porosity levels, i.e. nanoporosity and macroporosity, were induced in electrodeposited films to maximize the functionality. The nanomechanical properties were studied by nanoindentation, magnetic properties by vibrating sample magnetometry, and the magnetostriction was studied by X-ray diffraction applying an in-situ magnetic field. The results demonstrate a larger magnetic-field-induced crystal deformation in porous films compared to their fully-dense counterparts. The observed effects in porous Fe-Ga films are very appealing for the design of various strain-engineered nanomaterials, e.g., energy transducers or magnetoelectric composites.

*Acknowledgements:* This work has received funding from the European Union's Horizon2020 research and innovation programme under the MSCA grant №892661–MAGNUS and partially from №778357- SMARTELECTRODES.

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"SMARTELECTRODES" Workshop: Smart metallic and semiconductor materials: synthesis, characterization, applications and challenges.

# W3-O5. $Mo_xS_y$-containing coatings for photo/electrochemical water splitting applications

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Hydrogen is considered a feasible alternative to fossil fuels due to its high energetical density and environmentally friendly characteristics, and electrochemical water splitting is an economical route to produce $H_2$. However, a catalyst is needed to lower the kinetic barrier of the hydrogen evolution reaction (HER). Molybdenum sulfide is a known electrocatalyst for HER [1], but also exhibits photocatalytic properties [2], which make it an interesting and versatile material.

In the experiments presented in this study $Mo_xS_y$-based materials have been used as either catalysts or co-catalysts for electrochemical water splitting. In its simplest form, cathodically electrodeposited amorphous $MoS_{2-x}$ was used to synthesize thin films on both 2D and 3D electrodes for HER electrocatalysis. These films were found to be highly active in acidic media, as the material has active sites that catalyze $H^+$ adsorption, which is then followed by electrochemical recombination to produce $H_2$. Additionally, anodically electrodeposited $MoS_x$ was used as a co-catalyst to enhance the photoelectrochemical properties of a $WO_3$+$MoS_x$ photoanode. It was found that the composite would generate higher photocurrents than $WO_3$ films. These composites could also perform as HER electrocatalysts, owing to the dispersion of the $MoS_x$ material on the film's surface. The photo-/electrocatalytic electrodes were comprehensively studied by non-stationary methods. Local electrocatalytic activity was also measured by scanning electrochemical microscopy. Overall, electrodeposited $MoS_2$ is a catalytically active and highly versatile material for heterogeneous water splitting applications.

*Acknowledgements:* This work has received funding from the European Union's Horizon2020 research and innovation programme under the MSCA grant №778357-SMARTELECTRODES and from the Vilnius University Junior Researcher project MSF-JM-6/2021.

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"SMARTELECTRODES" Workshop: Smart metallic and semiconductor materials: synthesis, characterization, applications and challenges.

# W3-O6. Nanomultilayer structures based on chalcogenide amorphous semiconductors: obtaining and applications

**Alexei Meshalkin**[1,*], Elena Achimova[1], Vladimir Abaskin[1], Alexandr Prisacar[1], Genadi Triduh[1], Natalia Tsyntsaru[1,2]

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Chalcogenide glasses (ChGs) nanomultilayer structures based on $As_2S_3$-Se were used for direct surface relief grating (SRG) formation by holographic recording. Grating recording process in $As_2S_3$-Se nanomultilayer structure for different grating period and long recording time was performed. Simulated diffraction efficiency kinetics curves showed good agreement with the experimental results Analyses of diffraction efficiency kinetics and AFM images of recorded SRG showed that grating period increasing led to the SRG depth increasing in linear way. It was revealed that SRG recording rate was characterized by non-linear behavior, while modulation depth remained approximately the same value for all gratings. Two distinct mechanisms of SRG recording in ChGs thin films are distinguished depending on the polarization of writing beams: small scalar SRGs induced by photoinduced volume change, and giant vectorial SRGs induced by lateral mass transport. The exponential change of thickness modulation was obtained by the analysis of diffraction efficiency kinetics.

*Acknowledgements:* This work has received funding from the ANCD projects (20.80009.5007.03 and 21.80013.5007.1M) and partially from European Union's Horizon2020 research and innovation programme under the grant №778357-SMARTELECTRODES.

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"SMARTELECTRODES" Workshop: Smart metallic and semiconductor materials: synthesis, characterization, applications and challenges.

# W3-O7. Electrodeposited Co-Mo Composites with Titania for the Hydrogen Evolution Reaction

**Cheng Wang**,[*,1] Elizabeth Podlaha-Murphy[1]

[1]*Department of Chemical & Biomolecular Engineering University, Potsdam, NY 13699 USA*

[*] *Tel. 01 315 268-6665, wangc4@clarkson.edu*

**Purpose**: Cobalt-molybdenum based alloys are known hydrogen evolution electrocatalysts, and perform best in alkaline electrolytes [1]. Recently we have shown that the addition of titania particles to create composite Co-Mo-$TiO_2$ and Co-Mo-P-$TiO_2$ enhances the hydrogen evolution reaction (HER) [2]. In order to better understand the impact of $TiO_2$ in both depositing these composites and then being used as a catalyst to evolve hydrogen, the local pH change was characterized.
**Materials and Methods**: The composites were electrodeposited onto copper electrodes. Deposition was galvanostatic over a range of current densities from a citrate-boric acid electrolyte at a pH of 6.7. The potential was measured to assess the partial current densities. SEM was used to verify nanoparticle inclusion. To monitor the local pH change at the electrode a copper mesh substrate was used in close vicinity to a flat-bottom pH probe following a cell design from the literature [3]. HER electrocatalysis was examined in a pH 14 NaOH electrolyte.
**Results**: During electrodeposition, the pH initially dropped followed by a pH rise with time that was not influenced by the presence of $TiO_2$. However, there was a significant change in the local pH when $TiO_2$ was present in Co-Mo-based electrocatalyst during the HER process. In the HER electrolyte, without $TiO_2$ particles present in the solid state, the local pH change during electrolysis followed an expected increase with time, while with embedded $TiO_2$ particles in the metal matrix, the local pH initially decreased slightly and remained constant.
**Conclusions**: The results suggest that the enhanced HER performance with $TiO_2$ in the alloy composite electrocatalyst is a consequence of the buffering of the local pH that occurs at high pH, but not in the pH range of the electrodeposition conditions.

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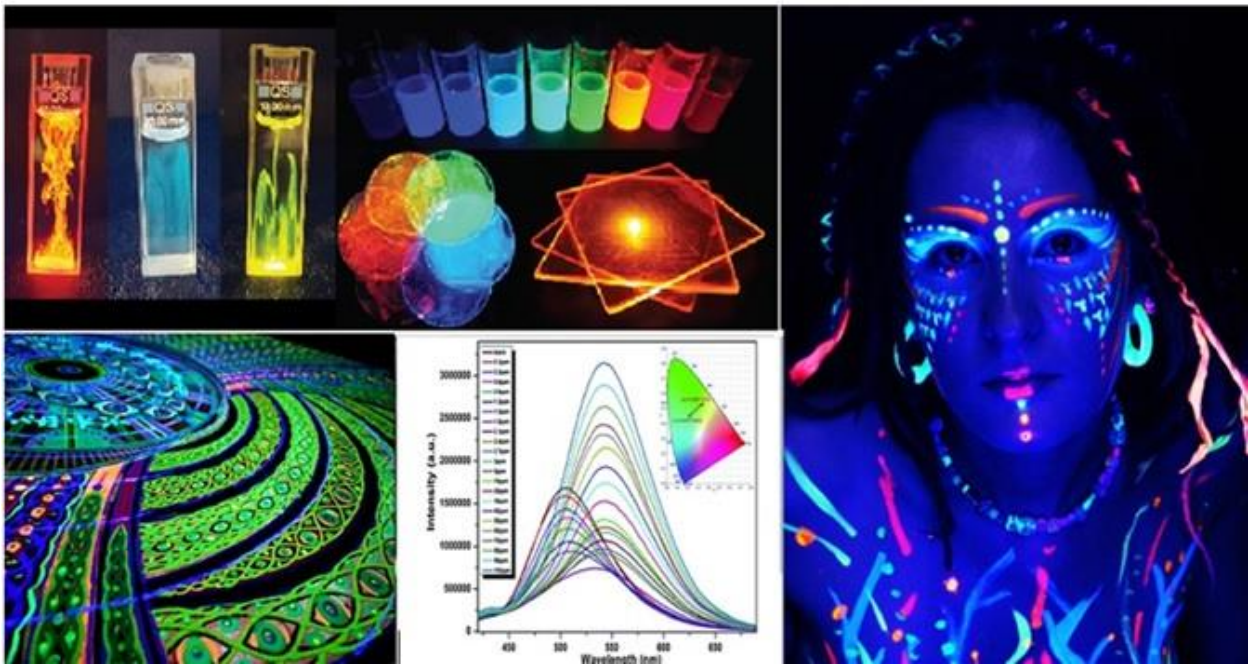
# Workshop 4

# Workshop on Optical Materials and their applications
# University of Aveiro, Portugal, July 5, 2022



The workshop of Optical materials in this broad overview covers the topics Optical Properties of Material Systems, The Materials Aspects of Optical Phenomena and the Materials Aspects of Devices and Applications.

Topics include but not limited to:

- Optical glasses and glass-ceramics
- Phosphor materials
- Upconversion materials
- Optical sensing materials
- Rare earth doped optically active materials
- Optically active Semiconductor materials
- Liquid crystals
- Photonic Materials
- Multifunctional materials with optical activity

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**Workshop on Optical Materials and their applications**
**University of Aveiro, Portugal,**
**July 5, 2022**

**Auditorium 3.**

**Morning session chair:**
**Dr. Suresh Kumar Jakka**
**i3n, Department of Physics, University of Aveiro, Portugal**

| | |
|---|---|
| **9.00-9:15** | WELCOME ADDRESS<br>Dr. Suresh Kumar Jakka, Dr. Pavani Krishnapuram and Dr. Igor Bdikin |
| **9:15-10:15** | **W4-PL1**<br>**Plenary Lecture**<br>**New advances in rare earth based pressure and temperature optical sensors**<br>**Prof. Victor Lavin**<br>*Laser and High-Pressure Spectroscopy group, University of La Laguna, Tenerife, Spain* |
| **10:15-10:45** | **W4-IT1**<br>**Invited talk**<br>**Development of new emitting optical fibers for mid-Infrared applications**<br>**Dr. Arnaud Lemiere**<br>*Photonic Glasses group, Tampere University, Finland* |
| **10:45-11:15** | **W4-IT2**<br>**Invited talk**<br>**Multifunctionality of Fluorescent 2D-BCNO Sheets**<br>Dr. Venkatramaiah<br>*SRM university, Chennai, India* |
| **11:15–11:30** | **Coffee break / Open discussions** |
| **11:30-12:00** | **W4-IT3**<br>**Invited talk**<br>**How to modify luminescent properties of materials by changing its structure**<br>**Dr. Bartosz Bondzior**<br>Photonic Glasses group, *Tampere University, Finland* |
| **12:00-12:15** | **W4-OP1**<br>**Oral presentation**<br>**Photocatalytic degradation activity of $SrTiO_3$ against Methylene Blue Dye**<br>**Mr. D. PrakashBabu**<br>*REVA university, India* |

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|---|---|
| **12:15-12:30** | **W4-OP2**<br>**Oral presentation**<br>**UV excited blue to green emitting $Tb^{3+}$ activated sodium calcium metasilicate color tunable phosphor for luminescent devices**<br>**Ms. Deepali**<br>*Delhi Technological University, India* |
| **12:30-12:40** | **W4-PP1**<br>**Poster presentation**<br>**Magnetically retrievable photocatalysis for dye degradation**<br>**Mr. Sachin Kulkarni**<br>*REVA university, India* |
| **12:40-12:50** | **W4-PP2**<br>**Poster presentation**<br>**Spectral investigation of thermally stable $Eu^{3+}$ activated potassium tungstate tellurite glasses for epoxy-resin free visible red component of photonic device applications**<br>**Mr. Vikas Sangwan**<br>*Delhi Technological University, India* |
| **12:50-13:00** | **W4-PP3**<br>**Poster presentation**<br>**Study on Photocatalytic inactivation of bacteria and dye degradation by Ag/$SiO_2$/ZnO based nanoparticles**<br>**Mr. Jaya Choudhary**<br>*REVA university, India* |
| **13:00–14:00** | **Lunch break** |
| | **Afternoon session chair:**<br>**Dr. Pavani Krishnapuram**<br>**I3n, Department of Physics, University of Aveiro, Portugal**<br>**And**<br>**Prof. K. Upendra Kumar**<br>**REVA University, Bangalore, India** |
| **14:00-15:00** | **W4-PL2**<br>**Plenary Lecture**<br>**A Method of Designing Uniform Sized Phosphor Nanoparticles and Fabrication of an AC-Electroluminescent Device**<br>**Prof. D. Haranath**<br>*Luminescent Materials and Devices (LMD) group, Department of Physics, National Institute of Technology Warangal, INDIA* |

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|---|---|
| **15:00-15:30** | **W4-IT4**<br>**Invited talk**<br>**Ceramic Luminescents for solid-state lighting applications**<br>**Dr Bungala Jamalaiah**<br>*RGUKT college of Engineering and Technology, Nandyal, India* |
| **15:30-16:00** | **W4-IT5**<br>**Invited talk**<br>**On thesis entitled "Cholesteric Liquid Crystal Emulsions for the Application in Anticounterfeiting Technology"**<br>**Mr. Buchaiah Gollapelli**<br>*Department of Physics, NIT Warangal, India* |
| **16:00-16:30** | **W4-IT6**<br>**Invited talk**<br>**Engineering of Silver Nanoclusters in Photoluminescent glass**<br>Dr. Seshadri Meruva<br>*K.G Reddy college of Engineering and Technology, Hyderabad, INDIA* |
| **16:30-16:45** | **W4-OP3**<br>**Oral presentation**<br>**Excitation and concentration-dependent energy transfer analysis in $Dy^{3+}$/$Eu^{3+}$ co-doped potassium zinc borophosphate glasses for white light emission**<br>Dr. R. Ramaraghavulu<br>*Annamacharya Institute of Technology and Sciences, Rajampet, India.* |
| **16:45-17:00** | **W4-OP4**<br>**Oral presentation**<br>**Enhancement of Photoluminescence of $CaSiO_3$:$Eu^{3+}$ co-doped $Dy^{3+}$ nanophosphor**<br>Prof. M. Madesh Kumar<br>*REVA University, India* |
| **17:00-17:15** | **W4-OP5**<br>**Oral presentation**<br>**Energy transfer and tunable emission from single phase triply doped $Ca_3Bi(PO_4)_3$ phosphor for WLEDs**<br>Mukesh K. sahu<br>*Delhi Technological University, India* |
| **17:15-17:30** | **Final discussion and comments** |

Workshop on Optical Materials and their applications

*Plenary Lecture*

# W4-PL1. New advances in rare earth based pressure and temperature optical sensors

**Víctor Lavín**[1,*], Marcin Runowski[1,2], and Ulises R. Rodríguez-Mendoza[1]

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Matter under extreme conditions of pressure (P) and/or temperature (T) is the subject of multidisciplinary studies involving physics, chemistry, materials science, biology or geology [1,2]. High P and low/high T conditions can be induced in a solid with the help of a diamond anvil cell for optical, vibrational, electrical, structural and/or magnetic studies. The determination of P-T within the hydrostatic chamber is a key issue that requires calibrated standards. Thanks to the transparency of diamonds to visible light, indirect in situ calibration can be performed by taking advantage of the high sensitivity to P and/or T changes of some rare earth (RE) emission lines in solids [1-3]. For pressure sensing applications, the shielding of 4f electrons of the RE in crystals produces very sharp emission lines in the optical range [3]. Less standardised is the method for measuring the exact temperature of the sample in the hydrostatic chamber. One technique is based on the existence of two emission levels of a RE ion close enough in energy to be considered in quasi-thermal equilibrium and whose relative population depends on T [3]. In this work we present different combinations of rare earth ions in different materials and nanomaterials that have been successfully tested as optical P- and/or T- sensors, along with the role of the host and the RE concentration.

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DOI: 10.1016/B978-0-12-816699-4.00010-4

Workshop on Optical Materials and their applications

***Plenary Lecture***

# W4-PL2. A Method of Designing Uniform Sized Phosphor Nanoparticles and Fabrication of an AC-Electroluminescent Device

**D. Haranath ***

*Luminescent Materials and Devices (LMD) group, Department of Physics, National Institute of Technology Warangal 506004, INDIA*
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In last few decades, several processes have been claimed worldwide for the synthesis of phosphor and aerogels separately for various applications including lighting, display, and insulated devices. Reference made to Kistler, S.S., 1931 (Nature- London, United States; Discovery of Aerogels: Coherent expanded aerogels and jellies), wherein it is suggested that solvent in a gel could be replaced by much rarer medium (i.e. gas) with little or no shrinkage. For the synthesis of gas-filled gels, the solvent from gels was displaced by other solvents of the low critical point. In the process, the gel (containing low critical temperature and pressure conditions of solvent) was placed in an autoclave with an excess of solvent, and the temperature was raised above its critical point to get gas-filled gel (i.e., an aerogel).

The current talk highlights a novel synthesis process using supercritical autoclave set-up for designing narrow size distribution of nanophosphor particles in the range 5 ± 2 nm, which could be easily commercialized. More particularly the current study relates to the synthesis of uniformly sized phosphor ($R_1$ $SiO_4$: $R_2$) particles, where $R_1$ relates to host metal, $R_2$ relates to dopant (transition and rare-earth metals) using tetraethylorthosilicate (TEOS), transition metal salts and rare-earth metals in varying ratio as dopant in oxidizing, reducing and inert surrounding media. Moreover, the as-synthesized phosphor aerogel finds many interesting and potential applications in the fields of display, lighting, insulating devices etc.

*Invited Talk*

# W4-IT1. Development of new emitting optical fibers for mid-Infrared applications

**Arnaud Lemiere** *

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Since the first demonstration of guiding light in an optical fiber, numerous works have been realized on the engineering of optical fibers to improve their optical and mechanical properties. Lately, a lot of work is, between others, focused on optical fibers for infrared (IR) applications like sensing and biomedical imaging. The motivation for working in IR comes from: 1- working in the infrared region requires more expensive and less easy-to-use devices, 2- the near-IR region is a transparency window for human skin and 3- the mid-IR region has strong molecules absorption bands. Considering the advantages of working in the IR region, it becomes interesting to develop optical fibers emitting light at different wavelengths in the IR from a laser source emitting at lower wavelength.

I will review in this talk the different studies I've realized in these last 5 years and the results I obtained for sensing and biomedical applications, by using two main techniques to generate new frequencies: IR supercontinuum generation [1,2,3] and rare-earth doping [4, 5].

The authors acknowledge the Academy of Finland, the European Union, and the region Bourgogne – Franche-Comte (France) for the financial support of my research work.

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Workshop on Optical Materials and their applications

*Invited Talk*

# W4-IT2. Multifunctionality of Fluorescent 2D-BCNO Sheets

**Venkatramaiah Nutalapati** * and Pratiksha Gawas

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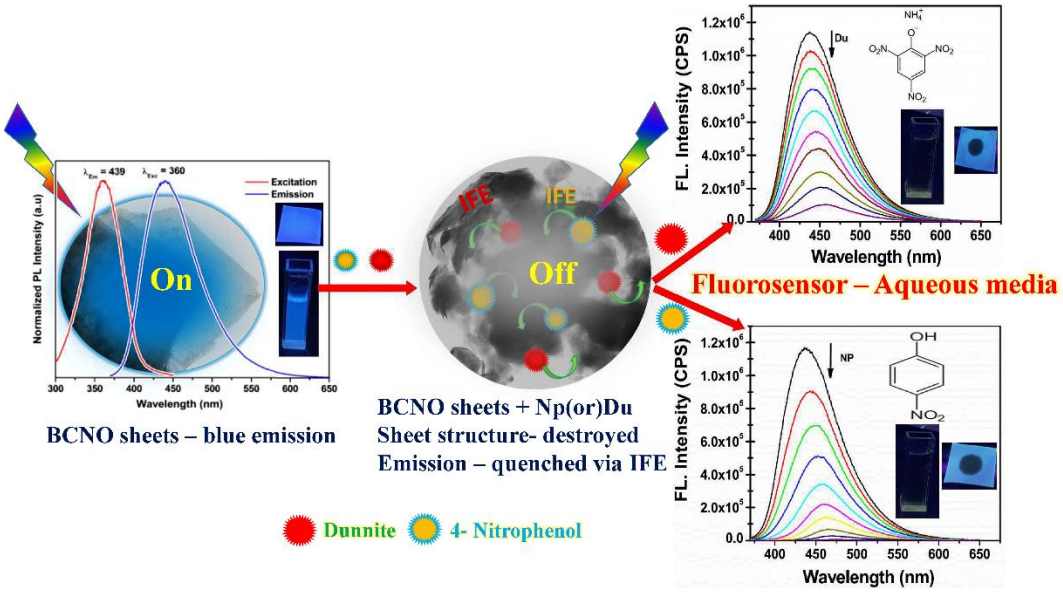
** Email:venkatrv1@srmist.edu.in*

Highly fluorescent 2D-BCNO (Boron carbon oxynitride) sheets synthesized *via* a new facile and simple approach for selective and sensitive detection of nitro-aromatic compounds namely 4-nitrophenol and Dunnite in aqueous medium. As synthesized 2D-BCNO sheets exhibit strong fluorescence emission in aqueous medium. Detailed photophysical properties and pH-dependent studies were explored. 2D-BCNO sheets showed a high fluorescence quenching towards explosive nitro-analytes and show an unprecedented selectivity for Dunninte and 4-nitrophenol. The remarkable sensitivity in the fluorescence quenching phenomena arises due to the unique Inner filter effect (IFE) and photo-induced electron transfer process through electrostatic interactions. The promising results from the real-time sample analysis with river and tap water as well as the interference studies in presence of other nitro-analytes elucidated the potential practical application of the sensor technology based on the 2D-BCNO sheets. Furthermore, the rapid and visual identification of Dunninte and 4-Nitrophenol at picogram levels with contact mode approach on solid substrates demonstrated that the introduced sensor technology is also suitable for onsite field analysis.

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Workshop on Optical Materials and their applications

***Invited Talk***

# W4-IT3. How to modify luminescent properties of materials by changing its structure

**Bartosz Bondzior**[1,2 *]

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The structural modifications are introduced to various crystals including silicates, borates and double-perovskites tungstates and molybdenates, as well as phosphate glasses, to obtain deserved impact on its luminescence.

In my talk I will present the results of my studies, where the structural modification was used to tune crucial properties of luminescent materials. The structural changes are introduced by substitution of host ions (in crystals) and changing the chemical composition (in glass).

The structural modifications of crystal and glass hosts can be used to impact the location of the dopant [1,2,3], to lower the symmetry of the crystal [4], to adjust the efficiency and the wavelength of the emission, to increase the thermal stability of luminescence [5] and to increase the sensitivity of the luminescence thermometers [5]. Besides its practical consequences, some theoretical models can also benefit from the results collected from these modified materials.

The research was conducted by Polish National Agency for Academic Exchange under the Bekker programme, project PPN/BEK/2020/1/00074.

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Workshop on Optical Materials and their applications

***Invited Talk***

# W4-IT4. Ceramic Luminescents for solid-state lighting applications

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Ceramic luminescents are an excellent alternative for modern lighting sources. They can be fabricated at a cheaper rate compared to that of currently available LEDs. They significantly reduce the production cost of automobile headlights, decorative illuminants, agricultural lighting sources etc. They show considerably greater durability due to their strength. Among the trivalent rare earths, the $Pr^{3+}$ ions can easily excited with the emission of blue-LED chip due to $Pr^{3+}$: $^3H_4 \rightarrow {}^3P_{2,1,0}$ excitation transitions. The $Pr^{3+}$ activated borate, aluminate and phosphate ceramic luminescents for various solid-state lighting applications were discussed.

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*Invited Talk*

# W4-IT5. Cholesteric Liquid Crystal Emulsions for the Application in Anticounterfeiting Technology

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Liquid crystals are highly responsive to external stimuli (such as electric field, magnetic field, heat, light, mechanical force and chemical analytes, etc.) of small magnitude which quantify them as smart material. Their ease of alignment along predetermined directions and facile orientation switching using small fields have made them attractive and successful in commercial applications. The inherent properties of cholesteric liquid crystals exhibit stimuli responsive configurations in the presence of chemical analytes, light and electric field which lead to the implementation in various biosensors and optical switching materials.

The scope of this research work is mainly to focus on preparation and characterization of fluorescent cholesteric liquid crystal (FCLC) emulsions which are synthesized in microfluidic approach. Cholesteric liquid crystals have been given fluorescent features either by the addition of synthetic carbon quantum dots or by naturally extracted chlorophyll dye. We describe the reflective and fluorescent features of FCLCs droplets to use in the field of anticounterfeiting technologies, such as security labels and authenticated/unauthenticated QR codes, by combining reflection and fluorescence phenomena.

Workshop on Optical Materials and their applications

*Invited Talk*

# W4-IT6. Engineering of Silver Nanoclusters in Photoluminescent Glass

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Silver (Ag) doped glasses have become attractive materials due to their usage in solid state displays, optical switching, bio and chemical-sensors, down-conversion of the solar spectrum and etc. [1-2]. The Ag nanoclusters have extremely small size, about a few nanometers, that can emit intense and broad luminescent band. Such a feature is absent in bulk silver due to its nature. The formation of Ag nanoclusters in various hosts (liquids, polymers and glasses) by the irradiation of x-ray and γ-ray, ion-irradiation, ion-exchange and laser writing has been reported in literature [3, 4]. Recently, Ag doped $SiO_2$+$Al_2O_3$+$CdF_2$+$PbF_2$+$ZnF_2$ glasses have been prepared using conventional melt-quenching technique [5]. They concluded that the glasses doped with Ag nanoclusters open a new perspective to prevent drawbacks that lead to the possibility of fabrication of bulk, thin films and fibers with improved structural and optical properties. Moreover, metallic particles (Ag, Au and Cu) coupled to rare earth (RE) in glass is the most successful proposal to overcome the quenching of fluorescence efficiencies for high RE ion concentrations. Therefore, engineering of silver clusters in glass materials have becom an attractive in solid state ligtining devices. In this talk, I am going to discuss glasses doped with Ag ions and Ag/$Eu^{3+}$ ions and have been successfully prepared by melt-quenching technique. The unique properties of excitation/emission of silver oxide embedded glass matrix, the inhomogeneous broadband character of B ($Ag^+$-$Ag^0$ pairs) and C ($Ag^+$-$Ag^+$ pairs) centers were identified upon 310 nm and 400 nm excitation wavelengths. The observed suppression of B center emission with extension of inhomogeneous broadening region toward the low energy side may be interpreted as due to non-radiative energy transfer process. The heat treated glasses show an energy transfer from B→C and Ag NP→B→C.

In Ag/Eu doped glasses, excitation spectra at 230, 250 nm and 355 nm exhibited broadband emissions in the UV and visible ranges (260 - 440 nm and 430 - 500 nm) which were associated to single $Ag^+$ ions and $Ag^+$- $Ag^0$ pairs. Moreover, enhancement of the $Eu^{3+}$ emission at 612 nm was observed with increasing Ag concentration. The effect was attributed to the energy transfer between Ag species and $Eu^{3+}$ ions, with a maximum enhancement factor of 4 times. Under 355 nm and 388 nm excitations, warm-white light and reddish-orange emissions were accomplished that may potentially be used in w-LEDs.

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Workshop on Optical Materials and their applications

***Oral Presentation***

# W4-OP1. Photocatalytic degradation activity of $SrTiO_3$ against Methylene Blue Dye

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In this work, we report synthesis of $SrTiO_3$ catalyst with efficient UV light driven photocatalytic activity towards methylene blue by modified solid state method. The surface morphology, phase purity, composition, and band gap of the prepared nanomaterials were studied using various analytical techniques. The band gap is 3.2 eV, and the crystalline structure is identified to be perovskite. The photocatalytic efficiency of perovskite $SrTiO_3$ catalyst was tested on the degradation of methylene blue (MB) under ultraviolet light irradiation. A 10 ppm MB dye solution in water was degraded by about 68% for $SrTiO_3$ catalyst at 120 min. this result demonstrates the photocatalyst efficiency of STO, which may be attributed to the band gap, high adsorbing of the dye molecules on the surface, large surface area, and low electron-hole recombination. In addition, STO demonstrated good photocatalytic degradation ability even after repeated cycles. Finally, an appropriate photocatalytic degradation mechanism was devised to indicate the photo-degradation function of STO.

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***Oral Presentation***

# W4-OP2. UV excited blue to green emitting $Tb^{3+}$ activated sodium calcium metasilicate color tunable phosphor for luminescent devices

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$Tb^{3+}$ doped $Na_4Ca_4Si_6O_{18}$ (NCMS: $Tb^{3+}$) phosphors have been synthesized via solid state reaction route with increasing in dopant concentration. The phase identification studies for NCMS: $Tb^{3+}$ phosphors have been done through X-ray diffraction (XRD) technique. The observed XRD patterns for as-synthesized phosphors shown satisfactory agreement with the standard pattern (JCPDS card no. 75-1687) of pure phase of $Na_4Ca_4Si_6O_{18}$ compound. The morphology and size of particles have been illustrated with scanning electron microscope (SEM) micrographs. The photoluminescence excitation (PLE) spectrum of $Tb^{3+}$ doped $Na_4Ca_4Si_6O_{18}$ phosphor depicts the strong excitation peak obtained in UV spectral region. The trivalent terbium activated NCMS phosphors excited under UV region (232 nm wavelength) exhibit intense emission in blue (350-470) and green (470-650) spectral regions. With increasing the concentration of $Tb^{3+}$ ions in host matrix, the emission color shifts from blue to green region due to cross relaxation energy transfer (CRET) mechanism and shows the tunable behaviour of $Tb^{3+}$ activated as-synthesized NCMS phosphor. The aforementioned results manifest that $Tb^{3+}$ activated sodium calcium metasilicate phosphor has an immense potential to contribute as a green and blue-green emitting component in lighting and display device applications.

Workshop on Optical Materials and their applications

***Oral Presentation***

# W4-OP3. Excitation and concentration-dependent energy transfer analysis in Dy3+/Eu3+ co-doped potassium zinc borophosphate glasses for white light emission

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Potassium zinc borophosphate (KZnBP) glasses containing $Dy^{3+}$, $Eu^{3+}$, and $Dy^{3+}/Eu^{3+}$ ions were prepared using the melt-quench method, and their photoluminescence properties were analyzed. The KZnBP glasses were co-doped with 0.5 mol% $Dy^{3+}$ and different concentrations of $Eu^{3+}$, and the ET mechanism between these ions was verified by excitation at 349, 364, 387 nm ($Dy^{3+}$), and 394 nm ($Eu^{3+}$). Under $Dy^{3+}$ excitation, the $Dy^{3+}/Eu^{3+}$ co-doped glass exhibited the characteristic emission peaks due to both ions. On the other hand, the intensities of the peaks at 480 nm ($^4F_{9/2}\rightarrow{}^6H_{15/2}$; blue) and 574 nm ($^4F_{9/2}\rightarrow{}^6H_{13/2}$, yellow) related to $Dy^{3+}$ decreased, and the $Eu^{3+}$ peaks at 591 nm ($^5D_0\rightarrow{}^7F_1$; red) and 617 nm ($^5D_0\rightarrow{}^7F_2$; orange) were intensified depending on the $Eu^{3+}$ concentration. This suggests that $Dy^{3+}$ sensitizes $Eu^{3+}$ ions. Based on the theories of Dexter and Reisfeld's approximation, the dipole-dipole interaction is responsible for energy transfer from $Dy^{3+}$ to $Eu^{3+}$ via the ET routes [$^4F_{9/2}$ ($Dy^{3+}$)+$^7F_{1,2}$($Eu^{3+}$)$\rightarrow{}^6H_{15/2}$($Dy^{3+}$)+$^5D_2$($Eu^{3+}$)] and [$^4F_{9/2}$ ($Dy^{3+}$)+ $^7F_0$($Eu^{3+}$)$\rightarrow{}^6H_{13/2}$($Dy^{3+}$)+$^5D_0$($Eu^{3+}$)]. The CIE coordinates of the $Dy^{3+}/Eu^{3+}$ co-doped glass are in the range of white light emission, highlighting the potential applications in warm white LEDs.

Workshop on Optical Materials and their applications

***Oral Presentation***

# W4-OP4. Enhancement of Photoluminescence of $CaSiO_3:Eu^{3+}$ co-doped $Dy^{3+}$ nanophosphor

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$CaSiO_3:Eu^{3+}$ co-doped $Dy^{3+}$ nanophosphor was synthesized by solution combustion technique. The nanocrystalline $CaSiO_3:Eu^{3+}$ co-doped Dy3+ (0-5 mol %) phosphors were synthesized by a low temperature solution combustion method by using Oxalyl dixyrazine (ODH) as a fuel and by fixing fuel to oxidizer ratios is unity [1-3]. In order to control the energy releasing during combustion, the stoichiometric composition of redox mixture are calculated. Analar grade Calcium Nitrate [$Ca(NO_3)_2.4H_2O$) Sigma Aldrich99.9%], Silica fumes[$SiO_2$ Sigma Aldrich 99.9%], Europium Nitrate [$Ce(NO_3)_3$ .$6H_2O$) Sigma Aldrich 99.9%], Dysprosium nitrate [$Dy(NO_3)_2$ , Sigma Aldrich 99.9%] and ODH ($C_2H_6N_4O_2$) prepared in lab were used as a starting materials. The stoichiometric amounts of Calcium Nitrate, Europium Nitrate, Dysprosium nitrate, Silica Fumes and ODH were taken in a crystalline dish and required quantity of double distilled water was added. The solution was continuously stirred for five minutes using a magnetic stirrer to get homogeneous redox mixture [4]. Then the solution was placed in a pre-heated muffle furnace maintained at 500˚C. The redox mixture undergoes thermal dehydration and auto-ignites with liberation of gaseous products. The combustion flame propagates throughout the redox mixture, the whole process was completed in less than 10 minutes and highly porous white nano-powders were obtained. These powders were grinded and sintered at 900˚ C for 3 hours The nanophosphors were characterized by X-ray diffraction (XRD), Fourier Transform Infrared spectroscopy (FTIR), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Photoluminescence (PL) of $Eu^{3+}$ and $Dy^{3+}$ co-doped CasiO3 nanophosphors were measured at room temperature. The effect of co-dopant on photoluminescence intensity has been studied. The optimized sample with 1 mol% Eu3+ doped $CaSiO_3$ and $Dy^{3+}$ co-doped 1 to 9 mole% samples were also investigated in details [5,6], the effect of Dy3+ co-doping concentrations luminescence intensity of $CaSiO_3$ samples can be tuned by adjusting the relative doping concentrations of the Dy3+ ions under a single wavelength excitation, which might find potential applications in the fields of light display systems, optoelectronic devices and white light emission LED.

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Workshop on Optical Materials and their applications

***Oral Presentation***

# W4-OP5. Energy transfer and tunable emission from single phase triply doped $Ca_3Bi(PO_4)_3$ phosphor for WLEDs

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Single phase multiple rare earth ions ($Tm^{3+}$, $Er^{3+}$, $Pr^{3+}$) activated $Ca_3Bi(PO_4)_3$ (CBP) have been synthesized via chemical co-precipitation method and scrutinize the various optical properties for the potential utility in advanced illuminating devices and optoelectronic applications. The diffraction patterns confirm the formation of single-phase cubic structure CBP samples and matched well with the standard data [1]. The reflectance spectrum shows the various absorption peaks owing to doped rare-earth ions. The micrographs show the asymmetrical micron size particles with some aggregation. The single ions doped CBP:$Tm^{3+}$ and CBP:$Er^{3+}$ phosphors emits intense blue and green near ultraviolet light source. The emission colors could be tuned with co-doped ($Tm^{3+}$, $Er^{3+}$) and tri-doped of ($Tm^{3+}$, $Er^{3+}$, $Pr^{3+}$) rare earth ions in CBP host materials. The warm white light emission was achieved under the excitation wavelength of 359 nm when the concentration of $Er^{3+}$and $Pr^{3+}$ ions were varied in optimized CBP:$Tm^{3+}$ phosphor. It was revealed that the energy was transferred from $Tm^{3+}$ to $Er^{3+}$ by overlap of the excitation spectra of $Tm^{3+}$ and $Er^{3+}$ ions. Whereas the energy transfer (ET) from the $Tm^{3+}$ to $Pr^{3+}$ ions via overlapping of emission spectrum of $Tm^{3+}$ ions with excitation profile of $Pr^{3+}$ ions in CBP host. The resonance-type ET from $Tm^{3+}$ to $Er^{3+}$ was confirmed to be via the dipole–dipole mechanism [2]. Hence, the mentioned structural and optical characteristics of the prepared single phase triply doped CBP:$Tm^{3+}$, $Er^{3+}$, $Pr^{3+}$ phosphor will find fascinating applicability as single-component phosphors in warm WLEDs.

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Workshop on Optical Materials and their applications

***Poster Presentation***

# W4-PP1. Magnetically retrievable photocatalysis for dye degradation

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Photocatalysts have been broadly applied in the degradation of organic chemicals utilizing and optimized to deliver productive, eco-freindly, and cheap materials for water treatment contaminated with dyes, and other natural contaminations. Over the most recent twenty years, materials which is magnetic in nature have emerged as most likely choice to work with heterogeneous catalysts in liquid phase. My interest of work is to synthesize magnetic materials using different synthesis processes accompanied by several modifications in order to enhance the photocatalytic efficiency, morphology, and reusability. The main significance of our research work is provided for different structures of catalysts which includes binary and ternary core-shell materials, multifunctional metal-organic framework materials, single-phase catalysts, and composites.

Workshop on Optical Materials and their applications

***Poster Presentation***

# W4-PP2. Spectral investigation of thermally stable $Eu^{3+}$ activated potassium tungstate tellurite glasses for epoxy-resin free visible red component of photonic device applications

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A transparent glass series of potassium tungstate tellurite (KTT) with varying $Eu^{3+}$ ions concentration was successfully synthesized by employing the conventional melt quenching method and their thermal, structural and luminescent features have been examined in detail. The amorphous or non-crystalline nature of prepared KTTEu glass samples were explored via XRD profiles. Using absorption spectra, the optical bandgap $(E_{opt})$ values for all prepared KTTEu glasses have been evaluated. PL emission spectra for as-prepared glass samples were achieved at 612 nm demonstrating red emission under n-UV and blue excitation source [1]. Under n-UV and blue excitation, all prepared KTTEu glasses are demonstrating red emission at 612 nm ascribed to $^5D_0 \rightarrow {}^7F_2$ transition and in which the intensity is increasing continuously with increasing the $Eu^{3+}$ ion concentrations up to 5.0 mol%. The activation energy (ΔE) and aggregate percentage loss in PL intensity around 86.87 % at 423 K have been evaluated for KTTEu50 glass matrix via temperature-dependent PL (TDPL) analysis showing the excellence in temperature stability of KTTEu glass matrix. All aforementioned results validate the $Eu^{3+}$ doped KTT glass samples have been auspicious candidates for the fabrication of organic epoxy-resin/binder-free red luminescent components in the domain of visible red laser and in the field of photonic device applications [2, 3].

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Workshop on Optical Materials and their applications

***Poster Presentation***

# W4-PP3. Study on Photocatalytic inactivation of bacteria and dye degradation by Ag/$SiO_2$/ZnO based nanoparticles

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Multifunctional nanoparticles are gradually attracting more and more Attention Because of their greater ability than conventional nanoparticles with various properties such as electronic, magnetic, optical and catalytic. Heterogeneous semiconductor based photocatalysis has received much attention across various disciplines as it offers an efficient and green solution for environmental problems [1 2]. In the present work we have paid attention on photocatalytic inactivation of *E coli* bacteria and Dye degradation by ZnO doped with Ag and/or Ln3+, ZnO@Ag and ZnO@Ag@$SiO_2$ Core and Core-shell nanoparticles synthesized via wet coprecipitation method. The structural characterization carried out by means of XRD, FTIR, SEM. The band gaps of these materials estimated with DRS. The photocatalysis efficiency has been enhanced by core-shell nanoparticles. The bacteria inactivation experimental results confirmed that the process of inactivation depends on the concentration of nanoparticles.

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# Company presentations

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# C1. Advanced nano-electrical characterization of solar cells and 2-D materials with Atomic Force Microcopy

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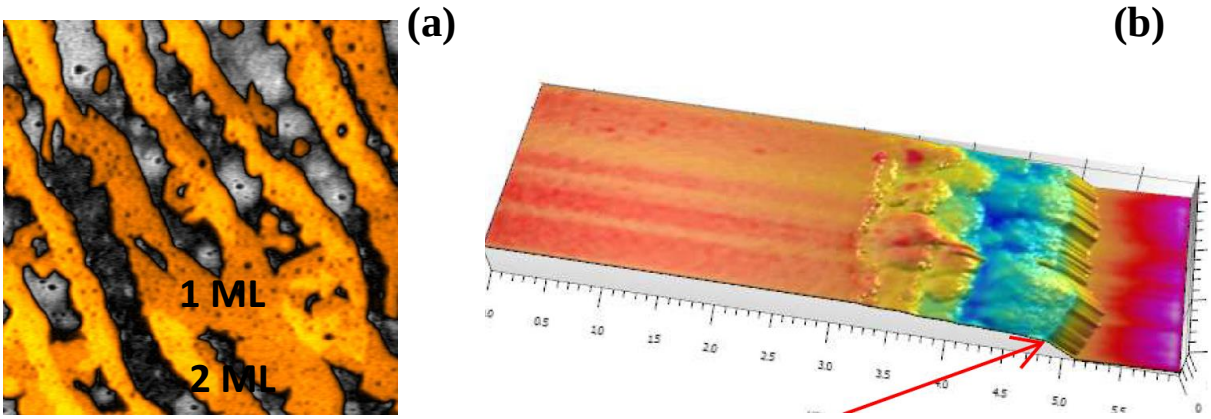
Over the past 30 years, Atomic Force Microscopy has evolved from a microscope to measure just the surface topography to a wide variety of measurement modes that provides a way to characterize other atomic interactions or physical properties like magnetic field, electric field, nanoscale dissipation processes, thermal conductivity, electrical conductivity, resistance, surface potential, piezoresponse, Young modulus,… Electrical nanocharacterization with AFM has emerged as a powerful tool to map electrical properties at the nanoscale, like surface potential (work function) and conductivity. However, traditional setups in AFM make difficult to obtain accurate and repeteable results over several types of samples.

In this contribution we will show the capabilities new developed AFM modes: High Definition Kelvin Force Microscopy (HD-KFM), ResiScope, Soft-Resiscope and Scaning Microwave that overcome the intrinsic difficulties of electrical nanocharacterization with AFM. This two techniques have been applied on a wide variety of substrates: bidimensional materials, like graphene or molibdene disulfide, organic and peruvskite solar cells or nanoparticles providing high stability, sensitivity and lateral resolution.




a) HD-KFM image on Graphene b) HD-KFM image of a cleaved perovskite solar cell.

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

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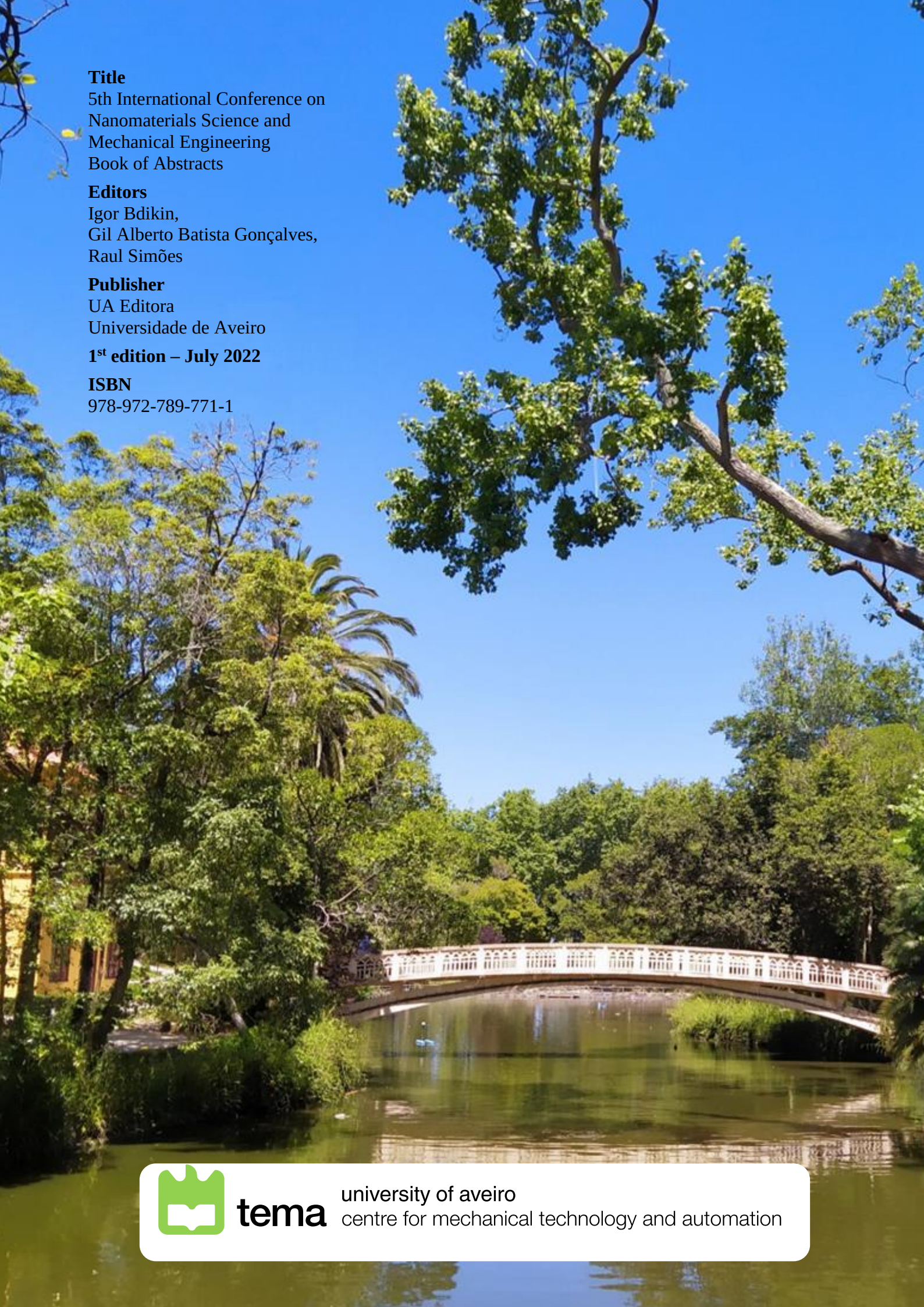
LASI establishes five inter-disciplinary research thematic lines to give response to social, scientific, health, sanitary, social, economic, and environmental challenges. The goal is to pave the next generation of knowledge and technologies for the development and transformation of the industry and society. 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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